Ligand-binding domain of the ultraspiracle (USP) protein

The invention relates to the spatial structure of the ligand-binding domain of the ultraspiracle protein, to the use of this structure for generating protein models of this protein in various conformations and of related proteins, and to methods of finding ligands of the ultraspriracle protein and of related proteins.

The ultraspiracle protein (termed USP hereinbelow) is the insect orthologue of the vertebrate retinoid X receptor (RXR). Like RXR, it belongs to the family of the nuclear receptors (NR). These nuclear receptors are located in the interior of the cell. They bind to responsive elements on the DNA as homo- or heterodimers and regulate the expression of genes. In order to be active they must bind specific small, frequently hydrophobic, ligands (for example steroids, retinoids, vitamin D). Nuclear receptors have a modular structure with functional domains for transactivation, DNA-binding and ligand-binding. While the DNA-binding domain of the nuclear receptors is highly conserved, the ligand-binding domains only show moderate homologies among each other. The spatial structures of various ligand-binding domains have already been determined (summary in 2) and allow an insight into the mechanism on which the activation is based, which comprises pronounced changes in the conformation of the ligand-binding domains. The binding of agonists leads to activation owing to the displacement of bound corepressors and the binding of coactivators, while the binding of antagonists prevents the interaction with the coactivator.

No spatial structures are available yet of insect nuclear receptors. In insects, for example the development from the larva to the adult insect is governed by nuclear receptors and involves the steroid hormone ecdysone and the isoprenoid juvenile hormone (3, 4, 5, 6). The ecdysone receptor, a nuclear receptor composed of two different subunits, EcR and USP, plays a key role in this process (7, 8, 9). It has been

known for a long time that the hormone ecdysone (in its active form 20-hydroxy-ecdysone) acts as ligand for the EcR subunit.

The ecdysone receptor constitutes an important insecticide target. If it is activated outside the windows in the period provided for insect development, this leads to severe damage or even to the death of the insects. The insecticidal action of ecdysone agonists is based on this mechanism (10, 11). Non-steroidal ligands of the EcR sub-unit which act specifically on Lepidoptera are already being used commercially as in-secticides (12).

USP is an orphan receptor for which no ligand is known as yet. While various authors have assumed that USP constitutes a receptor for juvenile hormones, this has never been proven by actual experiments (9). Indeed, it has been assumed that USP has no ligand at all, as this is described for some other nuclear receptors known from animals.

It was therefore an object of the present invention to provide the spatial structure of the ligand-binding domain (termed LBD hereinbelow) of the USP and to describe the possible ligand-binding pocket.

The object was achieved by providing a USP-LBD in crystalline form and by successfully carrying out the X-ray structure analysis of the crystals thus obtained.

The crystalline LBD according to the invention is preferably an LBD of the Heliothis virescens USP. The LBD according to the invention especially preferably has an amino acid sequence shown in SEQ ID NO: 1.

The subject-matter of the present invention is also a crystalline complex of a USP-LBD with a ligand.

The LBD according to the invention preferably has the structure coordinates defined in Table 1. The three-dimensional structure was solved and fully refined with the aid of protein crystals which are accessible to X-ray structure analysis at high resolution by means of molecular replacement. Subject-matter of the present invention is thus also the three-dimensional structure of the USP-LBD which can be determined with the aid of these structure coordinates.

A ligand-binding pocket, into which – like in the case of the other known structures of nuclear receptors – the ligands bind, has been identified in the three-dimensional structure according to the invention of the USP-LBD described herein. This is the first actual confirmation for the fact that USP has a functional ligand-binding pocket.

Subject-matter of the present invention is furthermore a USP-LBD comprising a ligand-binding pocket which is defined by the amino acids LEU230, VAL238, PRO239, PHE242, LEU249, LEU291, ILE294, MET323, LEU331, GLN338, ALA339, VAL341, PHE345, SER431, HIS434, LEU435, PHE438 and LEU440 as shown in SEQ ID NO: 2 and Table 1.

Subject-matter of the present invention is furthermore a USP-LBD comprising a ligand-binding pocket defined by the amino acids LEU230, VAL238, PRO239, PHE242, PRO245, VAL246, LEU249, CYS250, GLY253, ASN287, LEU290, LEU291, ILE294, MET323, LEU325, LEU331, SER335, ALA336, GLN338, ALA339, VAL341, ILE344, PHE345, VAL348, SER431, HIS434, LEU435, PHE438 and LEU440 as shown in SEQ ID NO: 2 and Table 1.

Subject-matter of the present invention is furthermore a USP-LBD comprising a ligand-binding pocket which is defined by the above-described amino acids and in which one or more of these amino acids are mutated. These are preferably conservative mutations, where an amino acid is exchanged for an amino acid with similar physical properties.

Such conservative substitutions encompass variations in which an amino acid is replaced by another amino acid from amongst the following group:

1. Small aliphatic residues, nonpolar residues or residues of little polarity: Ala, Ser, Thr, Pro and Gly;
2. Polar, negatively charged residues and their amides: Asp, Asn, Glu and Gln;
3. Polar, positively charged residues: His, Arg and Lys;
4. Large aliphatic nonpolar residues: Met, Leu, Ile, Val and Cys; and
5. Aromatic residues: Phe, Tyr and Trp.

Preferred conservative substitutions can be seen from the following list:

Original residue	Substitution
Ala	Gly, Ser
Arg	Lys
Asn	Gln, His
Asp	Glu
Cys	Ser
Gln	Asn
Glu	Asp
Gly	Ala, Pro
His	Asn, Gln
Ile	Leu, Val
Leu	Ile, Val
Lys	Arg, Gln, His
Met	Leu, Tyr, Ile
Phe	Met, Leu, Tyr
Ser	Thr
Thr	Ser
Trp	Tyr, Phe
Tyr	Trp, Phe
Val	Ile, Leu

The three-dimensional structure described herein of a USP-LBD is of great importance for the search for ligands with practical application. Such ligands can be used, for example, as insecticides with a novel mechanism of action. The ecdysone/juvenile hormone-governed development is only found in invertebrates and not in vertebrates; thus, it constitutes an insecticidal mechanism which is safe for the user and the environment.

Using the three-dimensional structure according to the invention of the USP-LBD, databases which contain the structures of a large number of compounds can be screened

with the aid of established, automated computer protocols (virtual screening). Algorithms such as FLEXX (13) or GOLD (14) are examples which can be used for virtual screening. With this procedure, compounds can be identified whose three-dimensional structure makes it possible to enter the binding pocket and to bind there, for example by forming hydrogen bonds, by hydrophobic interaction, by electrostatic interactions, by van-der-Waals interactions or by dipole interactions. The compounds identified thus can be synthesized and then used as, for example, insecticides or as effectors in expression systems (gene switch) based on the USP.

Another application of the three-dimensional structure according to the invention of the USP-LBD is the generation of new ligands. To this end, structural formulae for new ligands are generated on the computer using this structure and with the aid of established *de-novo* design programs, and these new ligands can enter the binding pocket, where they can bind, for example by forming hydrogen bonds, by hydrophobic interaction, by electrostatic interactions, by van-der-Waals interactions or by dipole interactions. Examples of *de-novo* design programs which are possible are LUDI (15), LEGEND (16) or GROW (17). Compounds generated thus can be synthesized and then also be used as, for example, insecticides or as effectors in expression systems (gene switch) based on the USP.

The three-dimensional structure according to the invention of the USP-LBD also makes it possible to predict the three-dimensional structure of a USP-LBD from other organisms by means of modelling methods. Such protein models can be used in the same manner as the three-dimensional structure solved herein. Comparison of the differences in the amino acid sequences makes it possible to predict differences in the ligand-binding pockets of various organisms. This is of use when specific ligands are searched for for specific organisms, or, conversely, when it is precisely unspecific ligands that are searched for. In addition, the three-dimensional structure according to the invention can be used for establishing protein models of other nuclear receptors with related sequences.

The present invention encompasses in particular the following subject matters and methods:

A computer-readable data storage medium comprising a data storage material on which the structure coordinates of an LBD according to the present invention are stored.

A computer-readable data storage medium in a form which makes it possible to generate a three-dimensional image of an LBD according to the present invention on a computer screen.

A method of generating protein models of USP-LBDs, characterized by the computer-aided generation of a three-dimensional image of an LBD according to the present invention.

A method of generating protein models of USP-LBDs in an agonistic conformation, characterized by the computer-aided generation of a three-dimensional image of an LBD according to the present invention in an agonistic conformation.

A method of generating protein models of nuclear receptors which have homologies with USP-LBDs, characterized by the computer-aided generation of a three-dimensional image of an LBD according to the present invention with a mutated amino acid sequence.

A method for generating protein models of nuclear receptors which have homologies with USP-LBDs in an agonistic conformation, characterized by the computer-aided generation of a three-dimensional image of an LBD according to the present invention with a mutated amino acid sequence in an agonistic conformation.

A method of finding USP ligands, characterized by the following steps:

(a) the computer-aided generation of a three-dimensional image of an LBD according to the present invention, and

(b) the computer-aided (virtual) screening of databases which contain structural data of chemical compounds for those structures which are capable of undergoing specific interactions with an LBD according to the present invention.

A method of finding USP ligands, characterized by the following steps:

(a) the computer-aided generation of a three-dimensional image of an LBD according to the present invention, and

(b) the computer-aided modelling of chemical compounds with structures which are capable of undergoing specific interactions with an LBD according to the present invention.

A method of finding USP-LBD ligands in an agonistic conformation, characterized by the following steps:

(a) the computer-aided generation of a three-dimensional image of an LBD according to the present invention in an agonistic conformation, and

(b) the computer-aided (virtual) screening of databases which contain structural data of chemical compounds for those structures which are capable of undergoing specific interactions with an LBD in an agonistic conformation.

A method of finding USP-LBD ligands in an agonistic conformation, characterized by the following steps:

(a) the computer-aided generation of a three-dimensional image of an LBD according to the present invention in an agonistic conformation, and

(b) the computer-aided modelling of chemical compounds with structures which are capable of undergoing specific interactions with an LBD in an agonistic conformation.

A method of finding active compounds for crop protection, in particular chemical compounds which, owing to binding to an LBD according to the present invention, bring about the activation or inhibition of USP, with the following steps:

(a) carrying out one of the abovementioned methods for finding USP ligands,

(b) synthesizing the compound(s) identified as ligands, and

(c) detecting the bioactivity of the compound synthesized in step (b) by transactivation assays, displacement assays or bioassays.

A method of finding active compounds for crop protection, in particular chemical compounds which, owing to binding to an LBD according to the present invention in an agonistic conformation, bring about the activation or inhibition of USP, with the following steps:

(a) carrying out one of the abovementioned methods for finding USP-LBD ligands in an agonistic conformation,

(b) synthesizing the compound(s) identified as ligands, and

(c) detecting the bioactivity of the compound synthesized in step (b) by transactivation assays, displacement assays or bioassays.

A method of finding effectors for systems for the inducible expression of target genes by means of USP, with the following steps:

(a) carrying out one of the abovementioned methods for finding USP ligands,

(b) synthesizing the compound(s) identified as ligands,

(c) applying a compound synthesized in step (b) to host cells or host organisms which contain a USP-based expression system, and

(d) detecting an induction or inhibition of the expression system.

The use of an LBD according to the present invention or of a computer-readable data storage medium according to the present invention for finding active compounds for crop protection or effectors for the controlled expression of target genes in host cells or intact host organisms.

The present invention is described in greater detail with reference to the examples which follow.

Examples

Example 1

Protein expression and purification

The Heliothis virescens USP-LBD (AS Val-205 to Met 466) was cloned in a pET-15b expression vector as N-terminal fusion protein with a His-tag and overexpressed in the E. coli strain BL21(DE3). The cells were cultured in 2x LB medium at 37°C and induced for 2 hours with 0.8 mM isopropyl-β-D-thiogalactopyranoside at 24°C. The protein extract was purified over a cobalt chelate column with subsequent gel filtration over a Superdex 200 16/60 column. The His-tag was then removed by digestion with thrombin and the protein was removed by gel filtration. A homogeneous monomeric protein species was present in the solution and was confirmed by means of SDS and native polyacrylamide gel electrophoresis and by denaturing and native electrospray ionization mass spectrometry.

Crystallization

Crystallization was effected by gas diffusion on hanging drops. The protein concentration employed was 3-9 mg/ml. Crystals 200 x 200 x 400 mm^3 in size formed within 10 days from a solution containing 10% of polyethylene glycol (PEG) 4000, 50 mM Tris (pH 7.5), 100 mM NaCl and 5 mM dithiothreitol and which was equilibrated in the reservoir against a solution of 20% polyethylene glycol (PEG) 4000 and 100 mM Tris (pH 7.5). The crystals belong to the tetragonal $P4_322$ spatial group with one monomer per asymmetric unit. The parameters of the standard cell are a=58.21 Å, b=58.21 Å, c=144.69 Å and $\alpha=\beta=\gamma=90°$. The solvent content is 32%, and the B-factor estimated in the Wilson Plot is 27 $Å^2$.

Data gathering, structure determination and refining

Crystals were immersed briefly in a 10% glycerol solution and shock-frozen in liquid nitrogen. The native data set was produced with a single crystal at measuring station ID14-EH2 at the ESRF (Grenoble, France). The data were processed with the aid of HKL programs (18). The crystal structure was solved by the molecular replacement method (19) by means of a partial hRXRα structure (20) as search model. A poor solution was achieved with a correlation of 24.8% and R_{free}=54.5% after refining as a rigid body. The phasing power of the model was low and required a number of manual generateing cycles with O (21). The wARP method (22) was used to verify the correctness of the partially-built structures. Refining was performed with CNS (23) using a maximum likelihood target function and solvent correction. Cycles of manual modelling and least-square minimization with subsequent simulated annealing and individual anisotropic B-factor refining gave rise to the final model. Solvent molecules were contoured in an $F_o - F_c$ map at a surface of 3σ. The final model, refined to a resolution of 1.65 Å, comprises 246 amino acid residues, 259 water molecules and one ligand molecule. A large portion of the connecting loop between Helix H5 and the beginning of the β-pleated sheet (amino acid residues 306-315) and the C-terminal extension of H12 (amino acid residues 459-466) could not be shown, owing to the poor electron density in these regions. The quality of the final model was checked with Procheck (24).

Characterization of the USP-LBD crystals by electrospray time-of-flight mass spectrometry (ESI TOF-MS) under natural conditions shows a heterogeneous mass distribution around 740 ± 50 Da in addition to the peak of the pure protein (30.2 kDa). This suggested that a ligand is present which is bound in LBD. The presence of a ligand was confirmed by the electron density. Various complementary techniques were used to characterize the ligand. The ligand, which is located in the binding pocket of the USP-LBD, was characterized as a phospholipid molecule. A phosphatidylglycerol or a phosphatidylethanolamine or a phosphatidylcholine would match the crystallographic data and are consistent with the results from mass

spectroscopy and chemical analysis. These amphiphilic molecules have a head group consisting of a phosphorylglycerol or a phosphorylethanolamine group and a tail of two different fatty acids which are bonded to the glycerol-3-phosphate by ester bonds. A detailed description of the ligand and its interactions with the USP-LBD residues are given in the following text.

Example 2

Architecture of the Heliothis virescens USP-LBD

In general, the architecture of the USP-LBD exhibits canonic NR folding with 11 α-helices (H1, H3-H12) and two short β-strands (s1-s2). This structure was compared with two other crystal structures which have essential properties of NRs and which are closely related to the Heliothis virescens USP: the binding pocket of agonist-bound RXRα (hRXRα/9-cis RA) and antagonist-bound mice RXRα (msRXRα/oleic acid). Superposing the USP-LBD with the structure of the holo-RXRα -LBD was carried out with the aid of a least-square fit [LSQ]. In total, the secondary structural elements of the USP-LBD are capable of reasonably good superposition by those of the holo-RXRα-LBD. The root mean square deviation (r.m.s.d.) is 1.22 Å for 183 out of 246 superposed Cα atoms. Seven helices are accessible to reasonably good superposition (r.m.s.d. 1.13, 0.88, 0.57, 1.18, 0.67, 0.69, 0.75 Å for H4, H5, H7-H11). The C-terminus of H1 is curved by approximately 2 Å relative to helix H3, and its r.m.s.d. is 1.63 Å. H3, H6 and the β-pleated sheet show larger deviations. The structure of the USP-LBD demonstrates that the activation helix H12 assumes a conformation which is similar to that of the antagonist-RXRα. The antagonistic AF-2 conformation of the USP-LBD is discussed further below.

The connecting loop L1-3 of most NRs usually behaves as a highly flexible region. In the case of hRXRα, the crystal structures of both the apo and the holo conformations show substantial differences in the regions which connect helices H1 and H3. In the holo-LDB structure, L1-3 consists of an extended loop which extends

beyone the β-pleated sheet and a Ω-loop. The apo form contains an additional helix in this region which unfolds in the holo-form. During the transition from the apo-form to the holo-form, L1-3 undergoes substantial movement. In particular, the Ω-loop becomes oriented towards the opposite side of the protein centre. As has been proposed on the basis of the comparison of the two structures, L1-3 might act as a molecular spring which accompanies the conformational changes which are linked to ligand binding. For the ligand-bound RARγ-LBD, the conformation of L1-3 resembles that of the holo-RXRα. Interestingly, L1-3 for ER-LBDs follows a path other than in the case of holo-RXRα. It runs between helix H3 and the β-pleated sheet, packed tightly to the protein centre.

In the case of the USP-LBD, L1-3 assumes none of the conformations which are otherwise found in the other NRs. Its course (Val-220 to Pro-239) was derived unambiguously from the electron density maps. Only few residues at the beginning of the loop, namely Asp-222, Pro-223 and Ser-224, were treated as alanins owing to the poor electron density of the side chains. The temperature factors of these residues are therefore higher (60-64 $Å^2$) than those of the other amino acids of L1-3 (on average 36 $Å^2$ over L1-3). The first residues of L1-3 form a path which crosses helix H3 in the region Gln-256 to Val-262. The next residues (Glu-226 to Pro-234) form an extended loop which runs along H3, and, finally, the last five residues of L1-3 (Asp-235 to Pro-239) form a loop which has substantial similarity with the Ω-loop observed in the LBDs of RXRα and RARγ. L1-3 assumes quite a tight conformation which makes it possible to establish direct contacts with the residues of helices H3, H11 and H12 and to stabilize their actual positions. This is important in as far as these helices are those structural elements which are subject to the greatest conformational changes owing to ligand binding.

The particular conformation of L1-3 is not based on crystal packing effects. In the region of the loop L1-3 of RXRα-LBD, the USP-LBD interacts with its symmetry-equivalent molecule via the β-pleated sheets. It is extremely likely that this interaction takes place since L1-3 does not already occupy this region when the protein is

in solution. If, owing to packing effects, L1-3 would be forced to swing and to move away from a conformation which is similar to the actual conformation of RXRα, several elements of the secondary structure would have to move drastically from this hypothetical conformation to their final position. It is therefore highly unlikely that this drastic reorganization of all of the LBD takes place, in particular because L1-3 lies in a region of the LBD in which L1-3 establishes very specific interactions with adjacent elements of the secondary structure.

Directly linked to loop L1-3, helix H3 differs from its counterparts in RXRα both regard to length and with regard to the position of the N- and C-terminal portion . In Heliothis virescens USP, H3 starts at Pro-240 and is therefore one turn longer than H3 in the ligand-bound RXRα (start at RXRα-Pro-264). The residues of H3 in the middle portion of the helix assume almost identical positions compared with the positions of the corresponding residues in the apo- and holo-RXRα-LBDs. However, both N- and C-terminal regions are curved towards the exterior of the protein centre. The N-terminal region of H3 (Pro-240 to Cys-250) is shifted substantially towards H11. It is tilted by approximately 24° in comparison with the same region in the holo-RXRα (approx. 7.2 Å between USP-Pro-245 and holo-RXRα-Pro-264). This position lies between those of the N-terminal regions in the apo-RXRα and the holo-RXRα-LBD structure. The outwardly curved C terminus of H3 (by approx. 10°) has effects on the arrangement of the adjacent loops L3-4 and L8-9. Loop L3-4, which is part of the signature region of NRs, is shifted laterally by approximately 1.8 Å and curved towards L8-9, while loop L8-9 itself is shifted outwardly by approximately 1.5 Å.

Example 3

The ligand-binding pocket

The ligand-binding pocket of Heliothis virescens USP is formed by residues of loop L1-3, helices H3, H5, H6 and H7, the β-pleated sheet and loop L11-12. As described

above, the N-terminal portion of helix H3 is markedly shifted outwardly compared with its opposite number in RXRα. Two other secondary structures which contribute to the binding pocket also differ from those in RXRα: 1) Helix 6 has moved inwardly by approximately 1.9 Å, and 2) the curvature of the β-pleated sheet points towards H1. The shift of the three structural elements which this entails lead to a widening of the ligand-binding pocket compared with that of the RXRα-LBD. The edge of the binding pocket is formed by the Ω-loop of L1-3, the N terminus of H3 and H6, while in the case of RXRα the opening of the pocket is formed by loop L11-12 and H6. At its opening, the binding pocket is approximately 13.5 Å wide (distance between Lys-241 in H3 and Gln-338 in H6). This opening is much wider than in the case of RXRα (7,1 Å from Pro-264 in H3 to Ala-340 in H6). The topology of the ligand-binding pocket is relatively unusual with a gap between H3 and H6. In RXRα and other NRs, this region forms fixed contacts with the connecting loop L1-3. The volume of the cavity of the USP-LBD achieves that of the hRXRα-LBD by a factor of 2.5 (1256 $Å^3$ in the case of USP compared with 489 $Å^3$ in the case of hRXRα).

Example 4

The putative ligand of USP in the crystal structure

Unexpectedly, the ligand-binding pocket of Heliothis virescens USP contains a molecule which was copurified and cocrystallized together with the USP-LBD. The fit of the electron density agrees well with the characterization of the molecules by mass spectroscopy and analytical chemistry. Similarly, recent crystallographic studies of the heterodimeric RARα/RXRα-LBD show an E.coli-endogenous oleic acid (C18) or a similar compound (stearic (C18) or palmitic (C16) acid) in the RXRα subunit. Even though this molecule is not the natural ligand of vertebrate NR, it induces and stabilizes an antagonistic AF-2 conformation which in all probability is very similar to the actual antagonist-bound RXRα.

In the present case, the best fit of the electron density was assumed with the assumption of a phospholipid whose first tail consists of a fatty acid with a length of 18 carbon atoms at C1 and a second chain at C2 which is 16 carbon atoms in length. The longer fatty acid of the two has a relatively twisted shape with two largish peaks, while the other fatty acid assumes a more normal form within the pocket. The tail of the phospholipid is hidden within the ligand-binding pocket. The glycerol moiety and the two fatty acids form van-der-Waals contacts with the residues in L1-3 (Leu-230, Val-238), H3 (Phe-242, Leu-249), H5 (Leu-291), L6-7 (Ala-339), H7 (Phe-345), H11 (Ser-431, His-434, Phe-438) and L11-12 (Leu-440). The head group of the phospholipid is positioned at the front at the opening of the pocket between H3 and H6. A strong hydrogen bond with Gln-338 (H6) is formed by the carbonyl group of the phosphorylglycerol in the case of phosphatidylglycerol and by the amino group of the ethanolamine in the case of phosphatidylethanolamine. In addition, an oxygen of the phosphate group is bound to a residue L1-3 (Cγ of Pro-239) by a hydrogen bridge.

It is assumed that the phospholipid found herein constitutes no natural USP ligands. However, it is shown unambiguously that USP ligands exist.

The residues which interact with the ligands are highly conserved within lepidopteran USPs, with the exception of Ser-431, which is replaced by a cysteine in msUSP. In contrast, among the 16 residues of the RXRα-LBD which interact with 9-cis RA, only 3 of the corresponding USP residues interact with the phospholipid (Leu-249, Ser-431 and His-434). The reason for this behaviour is mainly the different position of the ligands in the corresponding pockets. The 9-*cis* RA is very deep within the pocket, where its carboxylate group forms a salt bridge to Arg-316 of helix H5 of the hRXRα. In contrast, the phospholipid does not penetrate far into the inside of the pocket. For example the tail of the longer fatty acid lies approximately at atom C9 of 9-*cis* RA in hRXRα-LBD, while the tail of the other fatty acid extends almost to the β-ionone ring of 9-*cis* RA. As a consequence, Arg-297 does not participate in the anchorage of the ligand, as is observed in the case of the agonistic RXRα–, RARγ–

and other NR-LBDs. Nevertheless, it assumes almost the same position as Arg-316 of the holo-RXRα and not the position of the apo-RXRα conformation, which is exposed to the solvent. Instead of interacting with the ligand, Arg-297 forms hydrogen bonds with the backbone carbonyl group of Leu-325 (β-pleated sheet) and participates in a hydrogen bond network with Leu-290 (H5) and the side chain of Gln-256 (H3), with participation of water. In particular, two water molecules which are positioned spatially approximately at the two oxygen atoms of the carboxylate group of 9-*cis* RA participate in these interactions.

Example 5

The antagonistic conformation of the USP-LBD

The AF-2 domain in the structure of the USP-LBD exhibits an antagonistic conformation generated by the ligands in the ligand-binding pocket. H12 assumes the same conformation which has been found in the case of other antagonist-bound nuclear receptors such as RXRα /oleic acid, RARα/BMS614 and ER. In all these cases, it is observed that the groove in which H12 is positioned corresponds to the binding site for the helical nuclear receptor box of nuclear receptor coactivators. This helical nuclear receptor box is distinguished by the consensus sequence LXXLL, as has been shown for the ligand-binding domain of PPARγ, TRβ and ERα. In the case of the Heliothis virescens USP, Ile-450, Ala-453 and Leu-454 of H12 are approximately in the same position as the first, second and third leucin residue of the LXXLL binding motif (IXXAL instead of LXXLL). As in other antagonistic conformations of nuclear receptors, H12 is packed into a groove of residues of H3 and H4 and of L3-4 (Val-261, Arg-265, Met-275, Glu-276, Ile-279, Ile-282, Lys-283). However, in the case of the USP-LBD, L1-3 is also involved in the groove entopology and, with the residues Phe-227, Gln-228 and Phe-229, has van-der-Waals contacts with H12.

The length of H12 in the USP-LBD is identical to that of H12 in the antagonist-bound form of the RXRα-LBD. However, the structural principle which has been observed in another case of an antagonistic conformation of a nuclear receptor ligand-binding pocket is not found in its entirety in the case of the USP-LBD. Indeed, it has been found there that H11 coils up and thus permits H12 to bind to the binding groove of the nuclear receptor coactivator binding motif LXXLL. H11 is located in the extension of H10 and superposes very readily with H11 in the holo-RXRα-LBD structure, with the exception that the H11 of the USP-LBD is shorter by two residues. This is followed by a region 6 residues in length which connects H11 and H12 (His-439 to Thr-444). These amino acids of loop L11-12 span, in an extended conformation, a strand 12 Å in length. The C terminus of H11 contains three phenylalanins which are also found in RXRα. In apo-RXRα, the first two phenylalanins point towards the hydrophobic ligand-binding pocket while the third phenylalanin faces the solvent. In the agonist-bound form, the phenylalanins swap roles. In the USP-LBD, the situation is similar to the agonist-bound form of the RXRα-LBD: Phe-436 and Phe-437 face the solvent, while Phe-438 contributes to the ligand-binding pocket. In comparison with its counterpart in RXRα, the side chain of Phe-438 is rotated slightly and touches the ligand at the level of its shorter fatty acid. In the antagonist-bound form of RXRα, the first residue of the phenylalanin triplet corresponds to the end of H11. This residue is in approximately the position of the C-α atom of Phe-437. In the ligand-binding pocket, the two other phenylalanin residues, which are already part of L11-12, are orientated inwardly towards the inside of the protein. In a superposition of the Heliothis virescens USP and the antagonist-bound RXRα-LBD, these two residues collide with the phospholipid ligands.

Example 6

The connecting region L1-3 interacts with H3 and L11-12 and prevents an agonistic conformation

The binding of the phospholipid in the ligand-binding pocket of the USP-LBD probably generates important structural rearrangements in the USP-LBD. The comparison with apo- and holo-RXRα-LBD structures allows the assumption that in the USP-LBD, too, the molecular mechanisms which bring about the ligand-bound LBD conformation comprise the displacement of H3 and H11. However, in contrast to all other nuclear receptor LBDs known to date, the structural element L1-3 plays an essential role in the Heliothis virescens USP.

Loop L1-3 interacts with H3, H11, L11-12 and H12. These structural elements are most effective by the ligand binding. L1-3 stabilizes the N-terminus of H3 via a hydrogen bridge network with Arg-243 and Asn-254 of H3. The guanidinium moiety of the Arg-243 is anchored to the backbone carbonyls of Gly-233, Ser-236 and Val-238 by strong hydrogen bridges (distances 2.61, 2.97 and 2.78 Å, respectively) and shows a van-der-Waals contact with the side chain of Val-232. In addition, the backbone amide group of the Arg-243 is bound to the carbonyl group of Pro-239 (3.20 Å) by a hydrogen bond. The side chain of Asn-254 forms hydrogen bonds with the carbonyl group of Leu-230 (2.83 Å), to the amide group of Phe-229 (3.10 Å) and, via a water molecule, to the side chain of Gln-228. Moreover, it is in van-der-Waals contact with the carbonyl group of Phe-227. The backbone carbonyl group of Asn-254 forms a strong hydrogen bridge to the side chain of Glu-226 (2.74 Å).

L1-3 (Gln-228 to Arg-231, Asp-235 and Ser-236) is also in contact with N-terminal region of H11 and with L11-12. The backbone carbonyl group of Gln-228 forms a hydrogen bond with Ala-442 (3.20 Å), and the backbone carbonyl group of Phe-229 forms a strong hydrogen bridge with the amide group of Ala-442 (2.88 Å). In addition, Arg-231 stabilizes the loop L11-12 by means of strong interactions: the

backbone amide group forms a strong hydrogen bond with the carbonyl group of Leu-440 (2.90 Å), while the side chain forms a strong hydrogen bond with the carbonyl group of His-439 (3.00 Å) and shows van-der-Waals contacts with Val-441 and Ala-442. Other interactions concern the backbone carbonyl of Asp-235 with the side chain of His-439 and a water-mediated interaction with Val-441. The hydroxyl group of Ser-236 forms a van-der-Waals contact with the side chain of Leu-440.

It is important to state that a high degree of sequence conservation exists in all residues which participate in the interaction of L1-3 with H3 and with L11-12. The main interaction partners of H3, Arg-243 and Asn-254, are conserved strictly in all lepidopteran USPs. Likewise all interaction partners in L1-3 (Glu-226, Phe-227, Gln-228, Phe-229, Leu-230, Val-232, Gly-233, Ser-236, Val-238, Pro-239) are conserved strictly in all lepidopteran USPs, with the exception of Phe-227 and Phe-229, which are replaced by leucine and isoleucine in the Bombyx mori USP. In the case of the interactions of L1-3 with L11-12, too, the residues involved (L1-3: Gln-228 to Arg-231, Asp-235 and Ser-236; L11-12: His-439 to Ala-442) are conserved strictly in all lepidopteran USPs, with the exception of Phe-229 and Asp-235. This strongly suggests that interaction patterns of L1-3 with H3 and of L1-3 with L11-12 are similar in all lepidopteran USPs.

In the superposition of Heliothis virescens USP with the holo-RXRα-LBDs, it can be observed that some residues from L1-3 are approximately in the same position in the Heliothis virescens USP (Asn-237, Ser-236 and Phe-229), such as residues from L11-12 of holo-RXRα (Asp-444, Thr-445 and Phe-450). This comparison permits the informative conclusion that L1-3 in its actual conformation excludes the existence of an agonistic conformation since this would be hindered at loop L11-12. In any case, this is no crystallization artefact and reflects the particular role of this structural element in the lepidopteran USPs.

The sterical hindering of the agonistic position of H12 here is a constitutive component of the receptor structure and not the consequence of the bulky shape of

the ligand, as is the case in other nuclear receptor LBDs which are occupied by fully antagonistic ligands.

It can be predicted that ligand binding of agonists generates a change in the conformation of the USP-LBD, which makes L1-3, H12 and the other LBD residues which have been described jump into an antagonistic position.

In any case, this is not a crystallization artefact and constitutes the particular role of this structural element in the lepidopteran USPs.

Example 7

Agonistic conformation of the Heliothis virescens USP-LBD by homology modelling, based on the RXRα/9-cis-RA complex

In order to generate a 3D model of the Heliothis virescens USP-LBD, the lacking residues of the loop between helices H1 and H3 (L1-3) were complemented from the hRXRα crystal structure in such a way that a continuous backbone is formed. The resulting structure is the experimental hRXRα reference model.

Two hRXRα monomers were observed in the hRXRα standard cell, and the L1-3 region was poorly resolved in each of these monomers. Superposition of the two structures, which had been refined independently of one another, led to a suggestion as to where this loop should be modelled. A complete 3D model of hRXRα based on crystal structure and in which the residues in L1-3 are completed was built. The hydrogen atoms were completed with the aid of the Hgenerate option of the Charmm program.

The L1-3 region was relaxed by Powell minimization of the Charmm program (1000 optimization steps, dielectric constant : 4, gradient tolerance : 10^{-6}, step width 0.02, cutoff for non-binding interactions: 15 Å).

This optimized structure was used as template for the homology model of the Heliothis virescens USP-LBD.

The amino acid sequences of the Heliothis virescens USP-LBD and of hRXRα were assigned in accordance with Table 2.

With the aid of the software package Modeller and its standard settings, a 3D model was built with the aid of the assignment. The USP-LBD sequence shows a few insertions in loop 1-3 and in the loop before the first ß-pleated sheet. In order to establish meaningful conformations for these two regions, the option lego-loop of the software package O was used. The USP model structure was subsequently subjected to Powell minimization (2000 optimization steps, dielectric constant: 4, gradient tolerance: 10^{-6}, step width 0.02, cutoff for non-binding interactions: 15 Å). The quality of the structure thus obtained is analyzed with the program PROCHECK. Accordingly, 97% of the residues are in permitted regions and less than 2% of the residues are in prohibited regions. The latter are in the above-described modified regions.

Example 8

Comparison between the agonistic USP-LBD structure obtained from the hRXRα/9-cis RA complex and the USP-LBD crystal structure

The largest differences between these two structures are in the position of the activation helix (H12) and the path of the loop between the helices H1 and H3. The activation helix H12 is located in the experimental structure in the antagonistic position, while in the model structure it assumes an agonistic conformation which closes the ligand-binding niche. In the experimental structure, the loop L1-3 lies above the helix H3 and stabilizes the antagonistic position of H12 by hydrophobic contact. In contrast, this loop lies at a considerable distance from the central AFS-AD

helix in the agonistic homology model. Loop L1-3 is separated from helix H3 by the ß-pleated sheet.

Moreover, the size of the ligand-binding niche differs substantially between the two structures. The presence of the large fatty acid residue in the USP-LBD crystal structure causes a great cavity by shifting helices H3, H6 and H11. In the USP agonistic conformation, these helices are packed densely and produce a smaller ligand-binding niche.

The regions of the C-terminal ends of H3, H4, H5, H8 and H9 are rigid and capable of very good superposition in the two structures. In contrast, loop L1-3 and the C-termini of H3, H6 and H11 in the two structures are displaced relative to each other. These segments form the most mobile region of the ligand-binding domain of nuclear receptors. This movement is probably specific for each receptor and the ligand-generated displacement.

Information on the sequence listing

SEQ ID NO: 1 shows the amino acid sequence of the Heliothis virescens USP-LBD.

SEQ ID NO: 2 shows the amino acid sequence of the Heliothis virescens USP.

Information on the Tables

Table 1 shows the structure coordinates of the LBD of the Heliothis virescens USP.

Table 2 shows the amino acid sequence assignment for hRXRα and USP of Heliothis virescens and of further nuclear receptor LBDs for generateing a homology model of the agonistic USP conformation.

Table 1

REMARK coordinates from restrained individual B-factor refinement
REMARK refinement resolution: 20.0 - 1.65 A
REMARK starting r= 0.2151 free_r= 0.2506
REMARK final r= 0.2112 free_r= 0.2459
REMARK B rmsd for bonded mainchain atoms= 1.437 target= 1.5
REMARK B rmsd for bonded sidechain atoms= 2.272 target= 2.0
REMARK B rmsd for angle mainchain atoms= 2.299 target= 2.0
REMARK B rmsd for angle sidechain atoms= 3.310 target= 2.5
REMARK rweight= 0.1000 (with wa= 1.12122)
REMARK target= mlf steps= 30
REMARK sg= P4(3)22 a= 58.211 b= 58.211 c= 144.687 alpha= 90 beta= 90 gamma= 90
REMARK parameter file 1 : CNS_TOPPAR:protein_rep.param
REMARK parameter file 2 : CNS_TOPPAR:water_rep.param
REMARK parameter file 3 : eph.par
REMARK molecular structure file: alternate.mtf
REMARK input coordinates: anneal_2.pdb
REMARK reflection file= /home/billas/USP/SCALE0400/merge1A65/usp_20a1a65.10.cv
REMARK ncs= none
REMARK B-correction resolution: 6.0 - 1.65
REMARK initial B-factor correction applied to fobs :
REMARK B11= -1.985 B22= -1.985 B33= 3.970
REMARK B12= 0.000 B13= 0.000 B23= 0.000
REMARK B-factor correction applied to coordinate array B: -0.193
REMARK bulk solvent: density level= 0.33501 e/A^3, B-factor= 48.7849 A^2
REMARK reflections with |Fobs|/sigma_F < 0.0 rejected
REMARK reflections with |Fobs| > 10000 * rms(Fobs) rejected

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REMARK theoretical total number of refl. in resol. range:     30842 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |F|=0):   1417 (   4.6 % )
REMARK number of reflections rejected:                            0 (   0.0 % )
REMARK total number of reflections used:                      29425 (  95.4 % )
REMARK number of reflections in working set:                  26453 (  85.8 % )
REMARK number of reflections in test set:                      2972 (   9.6 % )
CRYST1   58.211   58.211  144.687  90.00  90.00  90.00 P 43 2 2
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REMARK VERSION:1.0
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ATOM      3  O   ALA   203     14.609  30.031  39.487  1.00 66.58
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ATOM     26  CA  GLU   207      7.970  23.165  43.644  1.00 49.47
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ATOM	35	CA	LEU	208	7.408	21.142	46.810	1.00	38.35
ATOM	36	CB	LEU	208	6.204	21.323	47.752	1.00	36.20
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ATOM	61	OE1	GLU	211	15.777	17.748	40.348	1.00	45.56
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ATOM	154	N	ALA	224	23.544	30.399	61.290	1.00	61.31
ATOM	155	CA	ALA	224	22.789	31.599	61.644	1.00	59.25
ATOM	156	CB	ALA	224	21.323	31.440	61.220	1.00	58.51
ATOM	157	C	ALA	224	22.878	31.880	63.143	1.00	58.07
ATOM	158	O	ALA	224	22.988	30.943	63.939	1.00	58.18
ATOM	159	N	GLU	225	22.844	33.159	63.528	1.00	56.07
ATOM	160	CA	GLU	225	22.909	33.507	64.950	1.00	54.05
ATOM	161	CB	GLU	225	22.498	34.969	65.221	1.00	54.53
ATOM	162	CG	GLU	225	22.700	35.401	66.703	1.00	55.83
ATOM	163	CD	GLU	225	21.439	35.872	67.407	1.00	56.62
ATOM	164	OE1	GLU	225	21.407	35.822	68.663	1.00	57.35
ATOM	165	OE2	GLU	225	20.464	36.314	66.743	1.00	57.42
ATOM	166	C	GLU	225	21.901	32.594	65.611	1.00	52.71
ATOM	167	O	GLU	225	20.737	32.557	65.201	1.00	52.66
ATOM	168	N	GLU	226	22.334	31.840	66.612	1.00	50.26
ATOM	169	CA	GLU	226	21.391	30.960	67.256	1.00	47.92
ATOM	170	CB	GLU	226	21.858	29.513	67.196	1.00	49.61

ATOM	171	CG	GLU	226	20.778	28.525	67.641	1.00	49.78
ATOM	172	CD	GLU	226	19.333	28.959	67.359	1.00	51.91
ATOM	173	OE1	GLU	226	18.452	28.312	67.956	1.00	50.08
ATOM	174	OE2	GLU	226	19.039	29.909	66.543	1.00	51.77
ATOM	175	C	GLU	226	21.015	31.344	68.670	1.00	46.28
ATOM	176	O	GLU	226	21.839	31.794	69.476	1.00	47.17
ATOM	177	N	PHE	227	19.733	31.155	68.942	1.00	41.52
ATOM	178	CA	PHE	227	19.138	31.503	70.206	1.00	38.73
ATOM	179	CB	PHE	227	17.723	32.022	69.963	1.00	40.03
ATOM	180	CG	PHE	227	17.640	33.061	68.876	1.00	40.91
ATOM	181	CD1	PHE	227	17.775	32.703	67.542	1.00	40.72
ATOM	182	CD2	PHE	227	17.464	34.402	69.192	1.00	42.62
ATOM	183	CE1	PHE	227	17.739	33.661	66.535	1.00	42.04
ATOM	184	CE2	PHE	227	17.426	35.374	68.188	1.00	42.27
ATOM	185	CZ	PHE	227	17.564	34.996	66.857	1.00	42.02
ATOM	186	C	PHE	227	19.119	30.339	71.174	1.00	34.83
ATOM	187	O	PHE	227	19.218	29.178	70.778	1.00	34.52
ATOM	188	N	GLN	228	18.982	30.687	72.445	1.00	33.69
ATOM	189	CA	GLN	228	18.979	29.735	73.540	1.00	32.01
ATOM	190	CB	GLN	228	19.290	30.468	74.847	1.00	34.80
ATOM	191	CG	GLN	228	20.680	31.080	74.935	1.00	39.39
ATOM	192	CD	GLN	228	21.768	30.029	74.916	1.00	40.63
ATOM	193	OE1	GLN	228	22.117	29.504	73.860	1.00	44.27
ATOM	194	NE2	GLN	228	22.301	29.706	76.093	1.00	42.65
ATOM	195	C	GLN	228	17.678	28.974	73.736	1.00	28.92
ATOM	196	O	GLN	228	17.035	29.174	74.750	1.00	28.29
ATOM	197	N	PHE	229	17.283	28.120	72.794	1.00	28.04
ATOM	198	CA	PHE	229	16.056	27.340	72.996	1.00	25.30
ATOM	199	CB	PHE	229	15.767	26.411	71.821	1.00	27.02
ATOM	200	CG	PHE	229	15.066	27.055	70.680	1.00	28.71
ATOM	201	CD1	PHE	229	15.599	28.170	70.052	1.00	28.96
ATOM	202	CD2	PHE	229	13.903	26.480	70.173	1.00	30.61
ATOM	203	CE1	PHE	229	14.991	28.708	68.918	1.00	29.32
ATOM	204	CE2	PHE	229	13.284	26.998	69.046	1.00	31.44
ATOM	205	CZ	PHE	229	13.829	28.117	68.412	1.00	31.43
ATOM	206	C	PHE	229	16.276	26.434	74.195	1.00	23.81

ATOM	207	O	PHE	229	15.385	26.202	75.014	1.00	22.15
ATOM	208	N	LEU	230	17.487	25.899	74.263	1.00	20.44
ATOM	209	CA	LEU	230	17.848	24.964	75.302	1.00	21.42
ATOM	210	CB	LEU	230	18.255	23.631	74.650	1.00	20.34
ATOM	211	CG	LEU	230	17.191	22.855	73.834	1.00	22.70
ATOM	212	CD1	LEU	230	17.860	21.762	73.013	1.00	23.14
ATOM	213	CD2	LEU	230	16.130	22.252	74.773	1.00	21.55
ATOM	214	C	LEU	230	19.017	25.540	76.094	1.00	20.71
ATOM	215	O	LEU	230	19.977	26.038	75.524	1.00	20.61
ATOM	216	N	ARG	231	18.931	25.467	77.411	1.00	20.48
ATOM	217	CA	ARG	231	20.018	25.997	78.211	1.00	20.62
ATOM	218	CB	ARG	231	20.023	27.525	78.176	1.00	20.50
ATOM	219	CG	ARG	231	18.907	28.184	79.017	1.00	24.52
ATOM	220	CD	ARG	231	17.560	28.025	78.342	1.00	27.62
ATOM	221	NE	ARG	231	16.465	28.674	79.060	1.00	28.14
ATOM	222	CZ	ARG	231	15.846	28.165	80.118	1.00	28.35
ATOM	223	NH1	ARG	231	16.208	26.986	80.598	1.00	27.27
ATOM	224	NH2	ARG	231	14.856	28.835	80.692	1.00	28.94
ATOM	225	C	ARG	231	19.957	25.585	79.663	1.00	20.62
ATOM	226	O	ARG	231	18.884	25.350	80.219	1.00	20.08
ATOM	227	N	VAL	232	21.138	25.549	80.265	1.00	20.70
ATOM	228	CA	VAL	232	21.276	25.244	81.684	1.00	23.23
ATOM	229	CB	VAL	232	22.596	24.499	81.961	1.00	24.57
ATOM	230	CG1	VAL	232	22.800	24.335	83.460	1.00	24.88
ATOM	231	CG2	VAL	232	22.565	23.135	81.289	1.00	23.34
ATOM	232	C	VAL	232	21.306	26.619	82.359	1.00	25.86
ATOM	233	O	VAL	232	22.284	27.349	82.225	1.00	29.87
ATOM	234	N	GLY	233	20.232	26.960	83.062	1.00	24.64
ATOM	235	CA	GLY	233	20.137	28.249	83.730	1.00	26.40
ATOM	236	C	GLY	233	20.170	28.129	85.240	1.00	27.72
ATOM	237	O	GLY	233	20.449	27.041	85.755	1.00	26.07
ATOM	238	N	PRO	234	19.863	29.206	85.980	1.00	28.00
ATOM	239	CD	PRO	234	19.340	30.507	85.515	1.00	30.45
ATOM	240	CA	PRO	234	19.886	29.158	87.447	1.00	28.48
ATOM	241	CB	PRO	234	19.772	30.627	87.833	1.00	30.42
ATOM	242	CG	PRO	234	18.804	31.123	86.802	1.00	32.04

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ATOM   243  C   PRO  234     18.752  28.323  88.037  1.00 27.91
ATOM   244  O   PRO  234     18.781  27.975  89.229  1.00 28.03
ATOM   245  N   ASP  235     17.757  27.996  87.210  1.00 26.13
ATOM   246  CA  ASP  235     16.636  27.186  87.680  1.00 23.93
ATOM   247  CB  ASP  235     15.333  27.686  87.064  1.00 28.77
ATOM   248  CG  ASP  235     15.405  27.820  85.544  1.00 31.24
ATOM   249  OD1 ASP  235     16.519  27.836  84.964  1.00 32.56
ATOM   250  OD2 ASP  235     14.327  27.922  84.919  1.00 34.70
ATOM   251  C   ASP  235     16.828  25.700  87.362  1.00 20.99
ATOM   252  O   ASP  235     16.019  24.881  87.751  1.00 19.94
ATOM   253  N   SER  236     17.914  25.369  86.666  0.50 20.63    AC1
ATOM   254  CA  SER  236     18.208  23.979  86.280  0.50 20.15    AC1
ATOM   255  CB  SER  236     19.196  23.969  85.111  0.50 19.44    AC1
ATOM   256  OG  SER  236     18.708  24.734  84.013  0.50 19.16    AC1
ATOM   257  C   SER  236     18.787  23.137  87.425  0.50 21.81    AC1
ATOM   258  O   SER  236     19.849  23.457  87.946  0.50 20.58    AC1
ATOM   259  N   ASN  237     18.125  22.037  87.782  1.00 21.94
ATOM   260  CA  ASN  237     18.621  21.202  88.886  1.00 25.34
ATOM   261  CB  ASN  237     17.498  20.331  89.450  1.00 30.84
ATOM   262  CG  ASN  237     17.020  19.301  88.472  1.00 34.04
ATOM   263  OD1 ASN  237     17.786  18.838  87.623  1.00 39.37
ATOM   264  ND2 ASN  237     15.748  18.913  88.588  1.00 39.05
ATOM   265  C   ASN  237     19.843  20.325  88.581  1.00 26.93
ATOM   266  O   ASN  237     20.180  19.405  89.339  1.00 32.05
ATOM   267  N   VAL  238     20.537  20.621  87.503  1.00 23.03
ATOM   268  CA  VAL  238     21.713  19.862  87.114  1.00 20.81
ATOM   269  CB  VAL  238     22.096  20.241  85.663  1.00 20.25
ATOM   270  CG1 VAL  238     23.336  19.495  85.207  1.00 19.20
ATOM   271  CG2 VAL  238     20.919  19.922  84.741  1.00 20.14
ATOM   272  C   VAL  238     22.844  20.185  88.106  1.00 20.62
ATOM   273  O   VAL  238     23.147  21.343  88.363  1.00 18.94
ATOM   274  N   PRO  239     23.428  19.153  88.719  1.00 20.32
ATOM   275  CD  PRO  239     23.144  17.726  88.541  1.00 20.40
ATOM   276  CA  PRO  239     24.515  19.328  89.688  1.00 21.49
ATOM   277  CB  PRO  239     24.911  17.892  90.023  1.00 22.13
ATOM   278  CG  PRO  239     23.696  17.174  89.847  1.00 20.51
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ATOM  279  C   PRO  239     25.663  20.039  89.023  1.00 24.59
ATOM  280  O   PRO  239     25.924  19.804  87.847  1.00 23.65
ATOM  281  N   PRO  240     26.388  20.879  89.777  1.00 24.92
ATOM  282  CD  PRO  240     26.142  21.311  91.167  1.00 26.02
ATOM  283  CA  PRO  240     27.524  21.603  89.202  1.00 26.88
ATOM  284  CB  PRO  240     28.222  22.161  90.438  1.00 26.73
ATOM  285  CG  PRO  240     27.039  22.543  91.299  1.00 29.18
ATOM  286  C   PRO  240     28.434  20.733  88.363  1.00 26.35
ATOM  287  O   PRO  240     28.847  21.125  87.259  1.00 27.72
ATOM  288  N   LYS  241     28.745  19.533  88.838  1.00 28.50
ATOM  289  CA  LYS  241     29.642  18.682  88.071  1.00 28.19
ATOM  290  CB  LYS  241     30.073  17.457  88.878  1.00 32.48
ATOM  291  CG  LYS  241     28.970  16.508  89.292  1.00 34.64
ATOM  292  CD  LYS  241     29.627  15.241  89.832  1.00 37.47
ATOM  293  CE  LYS  241     28.627  14.162  90.157  1.00 39.69
ATOM  294  NZ  LYS  241     29.359  12.932  90.578  1.00 42.50
ATOM  295  C   LYS  241     29.144  18.233  86.700  1.00 27.86
ATOM  296  O   LYS  241     29.935  17.790  85.868  1.00 27.57
ATOM  297  N   PHE  242     27.840  18.335  86.459  1.00 25.10
ATOM  298  CA  PHE  242     27.309  17.953  85.154  1.00 22.57
ATOM  299  CB  PHE  242     26.161  16.954  85.319  1.00 24.91
ATOM  300  CG  PHE  242     26.600  15.619  85.856  1.00 28.41
ATOM  301  CD1 PHE  242     27.411  14.790  85.102  1.00 30.20
ATOM  302  CD2 PHE  242     26.194  15.191  87.108  1.00 28.96
ATOM  303  CE1 PHE  242     27.813  13.544  85.583  1.00 31.58
ATOM  304  CE2 PHE  242     26.594  13.943  87.596  1.00 30.20
ATOM  305  CZ  PHE  242     27.400  13.127  86.832  1.00 32.03
ATOM  306  C   PHE  242     26.837  19.151  84.330  1.00 19.63
ATOM  307  O   PHE  242     26.386  18.991  83.190  1.00 20.79
ATOM  308  N   ARG  243     26.971  20.350  84.873  1.00 19.69
ATOM  309  CA  ARG  243     26.513  21.529  84.153  1.00 20.41
ATOM  310  CB  ARG  243     26.538  22.749  85.066  1.00 20.87
ATOM  311  CG  ARG  243     25.523  22.602  86.208  1.00 23.08
ATOM  312  CD  ARG  243     25.562  23.759  87.130  1.00 26.38
ATOM  313  NE  ARG  243     24.725  24.856  86.687  1.00 27.91
ATOM  314  CZ  ARG  243     23.394  24.873  86.728  1.00 28.35
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ATOM	315	NH1	ARG	243	22.697	23.825	87.192	1.00	26.91	
ATOM	316	NH2	ARG	243	22.764	25.975	86.343	1.00	28.11	
ATOM	317	C	ARG	243	27.238	21.813	82.846	1.00	20.13	
ATOM	318	O	ARG	243	26.596	22.114	81.836	1.00	19.71	
ATOM	319	N	ALA	244	28.564	21.734	82.838	1.00	20.90	
ATOM	320	CA	ALA	244	29.273	21.974	81.577	1.00	22.06	
ATOM	321	CB	ALA	244	30.773	21.896	81.796	1.00	21.20	
ATOM	322	C	ALA	244	28.842	20.984	80.492	1.00	21.05	
ATOM	323	O	ALA	244	28.527	21.365	79.366	1.00	21.57	
ATOM	324	N	PRO	245	28.783	19.696	80.822	1.00	21.63	
ATOM	325	CD	PRO	245	29.335	19.087	82.049	1.00	25.65	
ATOM	326	CA	PRO	245	28.377	18.672	79.861	1.00	22.28	
ATOM	327	CB	PRO	245	28.516	17.380	80.666	1.00	24.91	
ATOM	328	CG	PRO	245	29.614	17.694	81.605	1.00	25.26	
ATOM	329	C	PRO	245	26.943	18.859	79.329	1.00	19.49	
ATOM	330	O	PRO	245	26.691	18.778	78.118	1.00	21.31	
ATOM	331	N	VAL	246	26.013	19.123	80.230	1.00	20.18	
ATOM	332	CA	VAL	246	24.624	19.294	79.805	1.00	18.44	
ATOM	333	CB	VAL	246	23.693	19.269	81.028	1.00	18.35	
ATOM	334	CG1	VAL	246	22.221	19.536	80.620	1.00	18.11	
ATOM	335	CG2	VAL	246	23.766	17.845	81.678	1.00	17.69	
ATOM	336	C	VAL	246	24.501	20.568	78.968	1.00	18.23	
ATOM	337	O	VAL	246	23.773	20.603	77.977	1.00	18.23	
ATOM	338	N	SER	247	25.234	21.609	79.351	0.50	20.08	AC1
ATOM	339	CA	SER	247	25.198	22.858	78.599	0.50	21.19	AC1
ATOM	340	CB	SER	247	26.058	23.910	79.289	0.50	21.37	AC1
ATOM	341	OG	SER	247	25.484	24.292	80.517	0.50	23.67	AC1
ATOM	342	C	SER	247	25.712	22.621	77.189	0.50	21.32	AC1
ATOM	343	O	SER	247	25.180	23.161	76.217	0.50	21.62	AC1
ATOM	344	N	SER	248	26.756	21.811	77.076	1.00	20.43	
ATOM	345	CA	SER	248	27.322	21.502	75.766	1.00	21.62	
ATOM	346	CB	SER	248	28.541	20.594	75.916	1.00	24.31	
ATOM	347	OG	SER	248	29.660	21.350	76.354	1.00	24.89	
ATOM	348	C	SER	248	26.271	20.800	74.903	1.00	22.36	
ATOM	349	O	SER	248	26.158	21.061	73.697	1.00	22.32	
ATOM	350	N	LEU	249	25.513	19.895	75.519	1.00	22.35	

ATOM	351	CA	LEU	249	24.462	19.185	74.791	1.00	22.28
ATOM	352	CB	LEU	249	23.904	18.046	75.668	1.00	22.23
ATOM	353	CG	LEU	249	24.970	16.972	75.954	1.00	25.52
ATOM	354	CD1	LEU	249	24.441	15.919	76.922	1.00	26.39
ATOM	355	CD2	LEU	249	25.398	16.341	74.643	1.00	27.01
ATOM	356	C	LEU	249	23.358	20.152	74.352	1.00	21.63
ATOM	357	O	LEU	249	22.822	20.039	73.231	1.00	19.99
ATOM	358	N	CYS	250	23.012	21.102	75.217	1.00	21.10
ATOM	359	CA	CYS	250	21.995	22.098	74.856	1.00	21.22
ATOM	360	CB	CYS	250	21.701	23.044	76.019	1.00	20.65
ATOM	361	SG	CYS	250	20.853	22.249	77.396	1.00	22.08
ATOM	362	C	CYS	250	22.471	22.932	73.684	1.00	22.49
ATOM	363	O	CYS	250	21.687	23.302	72.828	1.00	23.08
ATOM	364	N	GLN	251	23.765	23.239	73.656	1.00	22.61
ATOM	365	CA	GLN	251	24.313	24.064	72.577	1.00	24.50
ATOM	366	CB	GLN	251	25.738	24.482	72.925	1.00	26.13
ATOM	367	CG	GLN	251	25.827	25.428	74.123	1.00	31.89
ATOM	368	CD	GLN	251	27.270	25.602	74.609	1.00	36.32
ATOM	369	OE1	GLN	251	28.146	26.020	73.846	1.00	38.70
ATOM	370	NE2	GLN	251	27.520	25.275	75.883	1.00	36.33
ATOM	371	C	GLN	251	24.290	23.309	71.255	1.00	23.96
ATOM	372	O	GLN	251	24.080	23.899	70.200	1.00	25.04
ATOM	373	N	ILE	252	24.506	21.998	71.323	1.00	23.74
ATOM	374	CA	ILE	252	24.475	21.143	70.140	1.00	24.05
ATOM	375	CB	ILE	252	24.877	19.690	70.493	1.00	25.71
ATOM	376	CG2	ILE	252	24.385	18.727	69.419	1.00	25.12
ATOM	377	CG1	ILE	252	26.405	19.596	70.658	1.00	26.17
ATOM	378	CD1	ILE	252	26.874	18.335	71.359	1.00	27.45
ATOM	379	C	ILE	252	23.032	21.183	69.642	1.00	25.30
ATOM	380	O	ILE	252	22.760	21.312	68.448	1.00	25.88
ATOM	381	N	GLY	253	22.101	21.105	70.580	1.00	25.76
ATOM	382	CA	GLY	253	20.698	21.167	70.213	1.00	24.72
ATOM	383	C	GLY	253	20.327	22.497	69.573	1.00	24.98
ATOM	384	O	GLY	253	19.611	22.527	68.561	1.00	24.56
ATOM	385	N	ASN	254	20.779	23.600	70.165	1.00	23.66
ATOM	386	CA	ASN	254	20.483	24.929	69.642	1.00	24.18

ATOM 387 CB ASN 254 21.063 25.999 70.566 1.00 23.04
ATOM 388 CG ASN 254 20.336 26.061 71.884 1.00 24.90
ATOM 389 OD1 ASN 254 19.147 25.729 71.954 1.00 22.87
ATOM 390 ND2 ASN 254 21.020 26.511 72.934 1.00 25.39
ATOM 391 C ASN 254 20.990 25.142 68.215 1.00 25.59
ATOM 392 O ASN 254 20.349 25.832 67.418 1.00 25.49
ATOM 393 N LYS 255 22.154 24.575 67.915 1.00 24.87
ATOM 394 CA LYS 255 22.718 24.669 66.572 1.00 26.12
ATOM 395 CB LYS 255 24.121 24.061 66.518 1.00 29.40
ATOM 396 CG LYS 255 25.162 24.983 67.112 1.00 33.68
ATOM 397 CD LYS 255 26.481 24.293 67.392 1.00 34.86
ATOM 398 CE LYS 255 27.280 24.027 66.150 1.00 35.57
ATOM 399 NZ LYS 255 28.719 23.853 66.527 1.00 33.75
ATOM 400 C LYS 255 21.816 23.924 65.608 1.00 26.04
ATOM 401 O LYS 255 21.539 24.415 64.507 1.00 25.57
ATOM 402 N GLN 256 21.358 22.741 66.009 1.00 24.02
ATOM 403 CA GLN 256 20.498 21.967 65.121 1.00 23.89
ATOM 404 CB GLN 256 20.325 20.546 65.658 1.00 25.47
ATOM 405 CG GLN 256 21.676 19.880 65.887 1.00 28.63
ATOM 406 CD GLN 256 21.565 18.517 66.534 1.00 30.93
ATOM 407 OE1 GLN 256 20.710 18.301 67.387 1.00 32.63
ATOM 408 NE2 GLN 256 22.439 17.599 66.149 1.00 30.18
ATOM 409 C GLN 256 19.156 22.658 64.915 1.00 24.45
ATOM 410 O GLN 256 18.596 22.598 63.828 1.00 24.20
ATOM 411 N ILE 257 18.662 23.338 65.942 1.00 23.21
ATOM 412 CA ILE 257 17.390 24.059 65.816 1.00 22.41
ATOM 413 CB ILE 257 16.895 24.535 67.180 1.00 20.26
ATOM 414 CG2 ILE 257 15.636 25.401 67.021 1.00 21.15
ATOM 415 CG1 ILE 257 16.607 23.298 68.039 1.00 22.12
ATOM 416 CD1 ILE 257 16.309 23.620 69.517 1.00 21.36
ATOM 417 C ILE 257 17.558 25.253 64.877 1.00 23.91
ATOM 418 O ILE 257 16.677 25.544 64.060 1.00 21.49
ATOM 419 N ALA 258 18.684 25.949 64.994 1.00 23.86
ATOM 420 CA ALA 258 18.939 27.081 64.103 1.00 25.37
ATOM 421 CB ALA 258 20.313 27.705 64.416 1.00 26.26
ATOM 422 C ALA 258 18.906 26.588 62.656 1.00 25.01

ATOM	423	O	ALA	258	18.306	27.238	61.783	1.00	25.91
ATOM	424	N	ALA	259	19.555	25.450	62.403	1.00	23.72
ATOM	425	CA	ALA	259	19.602	24.865	61.063	1.00	24.51
ATOM	426	CB	ALA	259	20.442	23.613	61.058	1.00	24.62
ATOM	427	C	ALA	259	18.187	24.525	60.623	1.00	24.36
ATOM	428	O	ALA	259	17.846	24.693	59.464	1.00	23.27
ATOM	429	N	LEU	260	17.374	24.015	61.544	1.00	23.02
ATOM	430	CA	LEU	260	15.986	23.685	61.188	1.00	24.75
ATOM	431	CB	LEU	260	15.237	23.070	62.366	1.00	26.22
ATOM	432	CG	LEU	260	15.550	21.633	62.742	1.00	31.27
ATOM	433	CD1	LEU	260	14.906	21.342	64.082	1.00	32.20
ATOM	434	CD2	LEU	260	15.054	20.679	61.658	1.00	33.32
ATOM	435	C	LEU	260	15.214	24.902	60.750	1.00	25.40
ATOM	436	O	LEU	260	14.391	24.821	59.834	1.00	23.40
ATOM	437	N	VAL	261	15.439	26.031	61.419	1.00	25.21
ATOM	438	CA	VAL	261	14.735	27.247	61.055	1.00	26.95
ATOM	439	CB	VAL	261	15.050	28.411	62.036	1.00	25.46
ATOM	440	CG1	VAL	261	14.386	29.700	61.544	1.00	27.40
ATOM	441	CG2	VAL	261	14.520	28.075	63.434	1.00	27.42
ATOM	442	C	VAL	261	15.104	27.671	59.640	1.00	26.53
ATOM	443	O	VAL	261	14.232	28.035	58.850	1.00	25.34
ATOM	444	N	VAL	262	16.396	27.611	59.320	1.00	27.29
ATOM	445	CA	VAL	262	16.874	27.995	57.993	1.00	28.11
ATOM	446	CB	VAL	262	18.430	27.910	57.905	1.00	30.08
ATOM	447	CG1	VAL	262	18.883	27.872	56.441	1.00	33.75
ATOM	448	CG2	VAL	262	19.051	29.104	58.606	1.00	32.97
ATOM	449	C	VAL	262	16.267	27.075	56.939	1.00	26.73
ATOM	450	O	VAL	262	15.909	27.511	55.840	1.00	26.28
ATOM	451	N	TRP	263	16.177	25.794	57.286	1.00	24.38
ATOM	452	CA	TRP	263	15.623	24.775	56.402	1.00	25.26
ATOM	453	CB	TRP	263	15.831	23.406	57.052	1.00	23.10
ATOM	454	CG	TRP	263	15.102	22.286	56.409	1.00	24.27
ATOM	455	CD2	TRP	263	13.881	21.697	56.873	1.00	24.86
ATOM	456	CE2	TRP	263	13.536	20.681	55.962	1.00	25.93
ATOM	457	CE3	TRP	263	13.051	21.936	57.974	1.00	24.53
ATOM	458	CD1	TRP	263	15.436	21.624	55.267	1.00	24.80

ATOM	459	NE1	TRP	263	14.501	20.655	54.990	1.00	27.16
ATOM	460	CZ2	TRP	263	12.391	19.895	56.115	1.00	26.26
ATOM	461	CZ3	TRP	263	11.911	21.151	58.132	1.00	23.32
ATOM	462	CH2	TRP	263	11.598	20.144	57.204	1.00	23.73
ATOM	463	C	TRP	263	14.125	25.047	56.175	1.00	24.66
ATOM	464	O	TRP	263	13.645	25.081	55.037	1.00	25.81
ATOM	465	N	ALA	264	13.391	25.278	57.252	1.00	24.56
ATOM	466	CA	ALA	264	11.949	25.506	57.103	1.00	25.04
ATOM	467	CB	ALA	264	11.304	25.733	58.464	1.00	26.00
ATOM	468	C	ALA	264	11.675	26.701	56.205	1.00	27.22
ATOM	469	O	ALA	264	10.838	26.640	55.293	1.00	24.71
ATOM	470	N	ARG	265	12.372	27.794	56.489	1.00	28.16
ATOM	471	CA	ARG	265	12.227	29.024	55.724	1.00	32.11
ATOM	472	CB	ARG	265	13.250	30.066	56.218	1.00	33.47
ATOM	473	CG	ARG	265	13.155	31.408	55.520	1.00	36.25
ATOM	474	CD	ARG	265	14.169	32.397	56.078	1.00	39.06
ATOM	475	NE	ARG	265	15.545	31.972	55.823	1.00	42.06
ATOM	476	CZ	ARG	265	16.609	32.534	56.391	1.00	43.94
ATOM	477	NH1	ARG	265	16.447	33.541	57.244	1.00	44.49
ATOM	478	NH2	ARG	265	17.827	32.092	56.110	1.00	43.52
ATOM	479	C	ARG	265	12.424	28.767	54.225	1.00	32.76
ATOM	480	O	ARG	265	11.843	29.460	53.392	1.00	35.61
ATOM	481	N	ASP	266	13.227	27.771	53.872	1.00	33.71
ATOM	482	CA	ASP	266	13.465	27.492	52.466	1.00	34.17
ATOM	483	CB	ASP	266	14.931	27.106	52.236	1.00	37.32
ATOM	484	CG	ASP	266	15.879	28.293	52.374	1.00	40.62
ATOM	485	OD1	ASP	266	15.556	29.392	51.866	1.00	40.66
ATOM	486	OD2	ASP	266	16.959	28.128	52.985	1.00	43.94
ATOM	487	C	ASP	266	12.544	26.447	51.833	1.00	33.93
ATOM	488	O	ASP	266	12.664	26.156	50.646	1.00	32.38
ATOM	489	N	ILE	267	11.640	25.869	52.619	1.00	32.18
ATOM	490	CA	ILE	267	10.694	24.897	52.077	1.00	30.21
ATOM	491	CB	ILE	267	9.820	24.279	53.210	1.00	29.16
ATOM	492	CG2	ILE	267	8.586	23.588	52.620	1.00	31.21
ATOM	493	CG1	ILE	267	10.643	23.291	54.038	1.00	29.01
ATOM	494	CD1	ILE	267	11.069	22.051	53.278	1.00	28.89

ATOM	495	C	ILE	267	9.800	25.670	51.093	1.00	30.06	
ATOM	496	O	ILE	267	9.256	26.715	51.421	1.00	29.41	
ATOM	497	N	PRO	268	9.653	25.164	49.862	1.00	31.41	
ATOM	498	CD	PRO	268	10.216	23.921	49.300	1.00	31.06	
ATOM	499	CA	PRO	268	8.813	25.857	48.879	1.00	31.62	
ATOM	500	CB	PRO	268	8.686	24.830	47.755	1.00	31.63	
ATOM	501	CG	PRO	268	10.012	24.126	47.811	1.00	34.16	
ATOM	502	C	PRO	268	7.459	26.286	49.444	1.00	31.83	
ATOM	503	O	PRO	268	6.762	25.483	50.051	1.00	31.61	
ATOM	504	N	HIS	269	7.128	27.566	49.267	1.00	31.08	
ATOM	505	CA	HIS	269	5.867	28.164	49.715	1.00	31.47	
ATOM	506	CB	HIS	269	4.677	27.277	49.300	1.00	33.82	
ATOM	507	CG	HIS	269	4.710	26.845	47.865	1.00	36.44	
ATOM	508	CD2	HIS	269	4.694	25.611	47.305	1.00	37.13	
ATOM	509	ND1	HIS	269	4.734	27.740	46.816	1.00	39.48	
ATOM	510	CE1	HIS	269	4.731	27.078	45.672	1.00	37.91	
ATOM	511	NE2	HIS	269	4.706	25.785	45.941	1.00	39.31	
ATOM	512	C	HIS	269	5.745	28.465	51.210	1.00	30.01	
ATOM	513	O	HIS	269	4.796	29.133	51.638	1.00	28.74	
ATOM	514	N	PHE	270	6.693	27.994	52.012	1.00	28.26	
ATOM	515	CA	PHE	270	6.607	28.222	53.454	1.00	27.87	
ATOM	516	CB	PHE	270	7.728	27.468	54.178	1.00	26.66	
ATOM	517	CG	PHE	270	7.661	27.563	55.684	1.00	24.18	
ATOM	518	CD1	PHE	270	6.867	26.683	56.415	1.00	24.15	
ATOM	519	CD2	PHE	270	8.385	28.536	56.372	1.00	26.34	
ATOM	520	CE1	PHE	270	6.792	26.775	57.822	1.00	22.45	
ATOM	521	CE2	PHE	270	8.316	28.637	57.778	1.00	24.45	
ATOM	522	CZ	PHE	270	7.516	27.754	58.494	1.00	23.03	
ATOM	523	C	PHE	270	6.650	29.707	53.811	1.00	28.65	
ATOM	524	O	PHE	270	5.866	30.175	54.634	1.00	29.19	
ATOM	525	N	SER	271	7.558	30.448	53.184	0.50	29.83	AC1
ATOM	526	CA	SER	271	7.676	31.876	53.463	0.50	31.34	AC1
ATOM	527	CB	SER	271	8.959	32.432	52.839	0.50	31.74	AC1
ATOM	528	OG	SER	271	10.104	31.869	53.460	0.50	31.64	AC1
ATOM	529	C	SER	271	6.458	32.663	52.974	0.50	32.85	AC1
ATOM	530	O	SER	271	6.301	33.839	53.296	0.50	33.99	AC1

ATOM	531	N	GLN	272	5.599	32.009	52.197	1.00	33.79
ATOM	532	CA	GLN	272	4.378	32.642	51.696	1.00	35.22
ATOM	533	CB	GLN	272	3.910	31.928	50.423	1.00	39.02
ATOM	534	CG	GLN	272	4.777	32.210	49.191	1.00	43.59
ATOM	535	CD	GLN	272	4.608	31.169	48.086	1.00	45.89
ATOM	536	OE1	GLN	272	3.488	30.794	47.727	1.00	47.68
ATOM	537	NE2	GLN	272	5.729	30.703	47.534	1.00	48.15
ATOM	538	C	GLN	272	3.255	32.633	52.742	1.00	35.20
ATOM	539	O	GLN	272	2.288	33.397	52.648	1.00	33.55
ATOM	540	N	LEU	273	3.383	31.756	53.736	1.00	33.18
ATOM	541	CA	LEU	273	2.402	31.651	54.811	1.00	31.26
ATOM	542	CB	LEU	273	2.695	30.398	55.653	1.00	30.14
ATOM	543	CG	LEU	273	2.671	29.015	54.988	1.00	29.04
ATOM	544	CD1	LEU	273	3.273	27.989	55.930	1.00	28.99
ATOM	545	CD2	LEU	273	1.231	28.638	54.645	1.00	29.21
ATOM	546	C	LEU	273	2.500	32.880	55.722	1.00	30.95
ATOM	547	O	LEU	273	3.556	33.513	55.793	1.00	30.58
ATOM	548	N	GLU	274	1.416	33.208	56.420	1.00	31.28
ATOM	549	CA	GLU	274	1.435	34.332	57.355	1.00	32.85
ATOM	550	CB	GLU	274	0.154	34.378	58.195	1.00	35.60
ATOM	551	CG	GLU	274	-1.039	35.022	57.511	1.00	40.50
ATOM	552	CD	GLU	274	-0.954	36.543	57.494	1.00	43.35
ATOM	553	OE1	GLU	274	-1.788	37.171	56.807	1.00	44.88
ATOM	554	OE2	GLU	274	-0.062	37.109	58.169	1.00	45.29
ATOM	555	C	GLU	274	2.615	34.079	58.287	1.00	32.91
ATOM	556	O	GLU	274	2.867	32.936	58.693	1.00	31.56
ATOM	557	N	MET	275	3.331	35.136	58.632	1.00	31.54
ATOM	558	CA	MET	275	4.483	35.010	59.507	1.00	31.78
ATOM	559	CB	MET	275	5.094	36.392	59.748	1.00	34.73
ATOM	560	CG	MET	275	6.288	36.403	60.673	1.00	37.61
ATOM	561	SD	MET	275	7.574	35.262	60.158	1.00	39.49
ATOM	562	CE	MET	275	7.940	35.869	58.496	1.00	39.54
ATOM	563	C	MET	275	4.149	34.351	60.838	1.00	31.91
ATOM	564	O	MET	275	4.885	33.474	61.305	1.00	31.90
ATOM	565	N	GLU	276	3.052	34.764	61.458	1.00	31.07
ATOM	566	CA	GLU	276	2.684	34.184	62.736	1.00	30.79

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ATOM   567  CB  GLU  276      1.499  34.938  63.341  1.00 35.06
ATOM   568  CG  GLU  276      1.866  36.382  63.755  1.00 37.66
ATOM   569  CD  GLU  276      3.043  36.434  64.731  1.00 40.34
ATOM   570  OE1 GLU  276      2.978  35.751  65.774  1.00 41.45
ATOM   571  OE2 GLU  276      4.034  37.157  64.464  1.00 42.59
ATOM   572  C   GLU  276      2.388  32.693  62.596  1.00 29.05
ATOM   573  O   GLU  276      2.529  31.946  63.559  1.00 28.93
ATOM   574  N   ASP  277      1.973  32.250  61.411  1.00 26.93
ATOM   575  CA  ASP  277      1.716  30.817  61.223  1.00 24.95
ATOM   576  CB  ASP  277      0.817  30.565  60.005  1.00 26.30
ATOM   577  CG  ASP  277     -0.656  30.768  60.320  1.00 26.04
ATOM   578  OD1 ASP  277     -0.984  31.102  61.476  1.00 29.19
ATOM   579  OD2 ASP  277     -1.492  30.596  59.410  1.00 26.42
ATOM   580  C   ASP  277      3.056  30.089  61.069  1.00 25.34
ATOM   581  O   ASP  277      3.226  28.967  61.579  1.00 25.43
ATOM   582  N   GLN  278      4.007  30.721  60.373  1.00 23.47
ATOM   583  CA  GLN  278      5.338  30.132  60.203  1.00 23.93
ATOM   584  CB  GLN  278      6.275  31.094  59.467  1.00 23.08
ATOM   585  CG  GLN  278      5.931  31.265  57.999  1.00 26.36
ATOM   586  CD  GLN  278      6.858  32.238  57.324  1.00 26.00
ATOM   587  OE1 GLN  278      8.075  32.122  57.439  1.00 26.10
ATOM   588  NE2 GLN  278      6.293  33.210  56.609  1.00 28.94
ATOM   589  C   GLN  278      5.917  29.850  61.588  1.00 22.78
ATOM   590  O   GLN  278      6.445  28.765  61.857  1.00 20.87
ATOM   591  N   ILE  279      5.821  30.849  62.461  1.00 23.32
ATOM   592  CA  ILE  279      6.322  30.719  63.825  1.00 22.80
ATOM   593  CB  ILE  279      6.125  32.046  64.591  1.00 24.62
ATOM   594  CG2 ILE  279      6.449  31.868  66.076  1.00 24.08
ATOM   595  CG1 ILE  279      6.997  33.125  63.943  1.00 27.52
ATOM   596  CD1 ILE  279      6.728  34.543  64.464  1.00 27.69
ATOM   597  C   ILE  279      5.638  29.560  64.573  1.00 22.81
ATOM   598  O   ILE  279      6.294  28.758  65.215  1.00 23.50
ATOM   599  N   LEU  280      4.318  29.463  64.498  1.00 20.16
ATOM   600  CA  LEU  280      3.653  28.382  65.186  1.00 18.30
ATOM   601  CB  LEU  280      2.125  28.553  65.113  1.00 19.64
ATOM   602  CG  LEU  280      1.589  29.739  65.931  1.00 22.60
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ATOM   603 CD1 LEU  280      0.093  29.931  65.623  1.00 24.59
ATOM   604 CD2 LEU  280      1.759  29.496  67.399  1.00 25.05
ATOM   605 C   LEU  280      4.045  27.028  64.653  1.00 17.14
ATOM   606 O   LEU  280      4.160  26.084  65.436  1.00 18.84
ATOM   607 N   LEU  281      4.225  26.905  63.335  1.00 17.52
ATOM   608 CA  LEU  281      4.586  25.591  62.773  1.00 19.05
ATOM   609 CB  LEU  281      4.550  25.618  61.241  1.00 19.60
ATOM   610 CG  LEU  281      3.167  25.782  60.595  1.00 21.40
ATOM   611 CD1 LEU  281      3.324  25.870  59.073  1.00 23.62
ATOM   612 CD2 LEU  281      2.266  24.621  60.975  1.00 21.20
ATOM   613 C   LEU  281      5.968  25.143  63.255  1.00 19.84
ATOM   614 O   LEU  281      6.164  23.977  63.620  1.00 19.38
ATOM   615 N   ILE  282      6.923  26.067  63.269  1.00 20.43
ATOM   616 CA  ILE  282      8.270  25.740  63.731  1.00 19.64
ATOM   617 CB  ILE  282      9.274  26.881  63.361  1.00 20.44
ATOM   618 CG2 ILE  282     10.619  26.706  64.102  1.00 20.04
ATOM   619 CG1 ILE  282      9.486  26.873  61.839  1.00 20.45
ATOM   620 CD1 ILE  282     10.278  28.076  61.323  1.00 22.03
ATOM   621 C   ILE  282      8.255  25.496  65.239  1.00 19.41
ATOM   622 O   ILE  282      8.894  24.574  65.717  1.00 19.21
ATOM   623 N   LYS  283      7.533  26.322  65.992  1.00 17.59
ATOM   624 CA  LYS  283      7.480  26.148  67.446  1.00 19.01
ATOM   625 CB  LYS  283      6.624  27.246  68.103  1.00 19.89
ATOM   626 CG  LYS  283      6.596  27.154  69.613  1.00 23.82
ATOM   627 CD  LYS  283      5.948  28.388  70.243  1.00 26.99
ATOM   628 CE  LYS  283      5.645  28.183  71.731  1.00 30.98
ATOM   629 NZ  LYS  283      6.837  27.917  72.599  1.00 34.38
ATOM   630 C   LYS  283      6.873  24.791  67.778  1.00 19.44
ATOM   631 O   LYS  283      7.274  24.120  68.729  1.00 19.31
ATOM   632 N   GLY  284      5.882  24.390  66.983  1.00 19.18
ATOM   633 CA  GLY  284      5.240  23.124  67.254  1.00 18.56
ATOM   634 C   GLY  284      5.981  21.885  66.806  1.00 18.31
ATOM   635 O   GLY  284      5.731  20.805  67.328  1.00 19.56
ATOM   636 N   SER  285      6.941  22.024  65.895  1.00 18.65
ATOM   637 CA  SER  285      7.633  20.844  65.384  1.00 17.51
ATOM   638 CB  SER  285      7.453  20.755  63.870  1.00 19.70
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ATOM	639	OG	SER	285	8.063	21.874	63.212	1.00	18.48
ATOM	640	C	SER	285	9.136	20.728	65.663	1.00	15.25
ATOM	641	O	SER	285	9.705	19.673	65.406	1.00	15.43
ATOM	642	N	TRP	286	9.770	21.759	66.203	1.00	15.99
ATOM	643	CA	TRP	286	11.221	21.642	66.395	1.00	16.28
ATOM	644	CB	TRP	286	11.812	22.920	67.007	1.00	17.10
ATOM	645	CG	TRP	286	11.458	23.226	68.414	1.00	17.32
ATOM	646	CD2	TRP	286	12.117	22.736	69.592	1.00	18.06
ATOM	647	CE2	TRP	286	11.440	23.291	70.709	1.00	20.12
ATOM	648	CE3	TRP	286	13.208	21.882	69.815	1.00	17.92
ATOM	649	CD1	TRP	286	10.445	24.033	68.850	1.00	18.61
ATOM	650	NE1	TRP	286	10.427	24.076	70.227	1.00	18.32
ATOM	651	CZ2	TRP	286	11.816	23.020	72.027	1.00	17.23
ATOM	652	CZ3	TRP	286	13.580	21.608	71.136	1.00	18.42
ATOM	653	CH2	TRP	286	12.889	22.172	72.219	1.00	19.75
ATOM	654	C	TRP	286	11.668	20.443	67.219	1.00	16.59
ATOM	655	O	TRP	286	12.655	19.766	66.886	1.00	17.31
ATOM	656	N	ASN	287	10.938	20.167	68.282	1.00	15.26
ATOM	657	CA	ASN	287	11.301	19.059	69.157	1.00	14.41
ATOM	658	CB	ASN	287	10.508	19.180	70.456	1.00	17.68
ATOM	659	CG	ASN	287	10.894	18.145	71.474	1.00	19.61
ATOM	660	OD1	ASN	287	11.757	18.374	72.348	1.00	23.92
ATOM	661	ND2	ASN	287	10.251	16.991	71.384	1.00	18.83
ATOM	662	C	ASN	287	11.096	17.718	68.448	1.00	14.74
ATOM	663	O	ASN	287	11.954	16.846	68.508	1.00	16.16
ATOM	664	N	GLU	288	9.966	17.555	67.752	1.00	15.22
ATOM	665	CA	GLU	288	9.745	16.319	66.986	1.00	16.77
ATOM	666	CB	GLU	288	8.367	16.358	66.288	1.00	17.55
ATOM	667	CG	GLU	288	7.213	16.044	67.224	1.00	18.68
ATOM	668	CD	GLU	288	5.868	16.134	66.548	1.00	23.02
ATOM	669	OE1	GLU	288	5.786	15.849	65.342	1.00	28.18
ATOM	670	OE2	GLU	288	4.887	16.461	67.243	1.00	29.07
ATOM	671	C	GLU	288	10.838	16.122	65.921	1.00	17.49
ATOM	672	O	GLU	288	11.338	15.014	65.743	1.00	16.93
ATOM	673	N	LEU	289	11.193	17.204	65.220	1.00	14.56
ATOM	674	CA	LEU	289	12.196	17.130	64.173	1.00	15.76

ATOM 675 CB LEU 289 12.248 18.451 63.390 1.00 14.77
ATOM 676 CG LEU 289 11.006 18.639 62.483 1.00 16.67
ATOM 677 CD1 LEU 289 10.932 20.093 62.002 1.00 18.25
ATOM 678 CD2 LEU 289 11.083 17.667 61.287 1.00 15.71
ATOM 679 C LEU 289 13.555 16.784 64.752 1.00 16.05
ATOM 680 O LEU 289 14.301 16.022 64.138 1.00 16.56
ATOM 681 N LEU 290 13.884 17.312 65.929 1.00 16.37
ATOM 682 CA LEU 290 15.190 16.951 66.529 1.00 16.68
ATOM 683 CB LEU 290 15.477 17.734 67.809 1.00 17.02
ATOM 684 CG LEU 290 15.786 19.219 67.684 1.00 22.29
ATOM 685 CD1 LEU 290 16.294 19.726 69.046 1.00 23.74
ATOM 686 CD2 LEU 290 16.865 19.454 66.604 1.00 25.08
ATOM 687 C LEU 290 15.229 15.471 66.868 1.00 16.18
ATOM 688 O LEU 290 16.214 14.803 66.605 1.00 17.45
ATOM 689 N LEU 291 14.142 14.958 67.465 1.00 16.16
ATOM 690 CA LEU 291 14.088 13.553 67.826 1.00 17.64
ATOM 691 CB LEU 291 12.828 13.289 68.666 1.00 17.32
ATOM 692 CG LEU 291 12.824 13.961 70.046 1.00 20.40
ATOM 693 CD1 LEU 291 11.405 13.964 70.627 1.00 22.18
ATOM 694 CD2 LEU 291 13.789 13.222 70.971 1.00 23.46
ATOM 695 C LEU 291 14.087 12.662 66.595 1.00 15.65
ATOM 696 O LEU 291 14.645 11.569 66.611 1.00 17.39
ATOM 697 N PHE 292 13.434 13.116 65.520 1.00 14.81
ATOM 698 CA PHE 292 13.360 12.330 64.311 1.00 15.62
ATOM 699 CB PHE 292 12.392 12.993 63.314 1.00 16.43
ATOM 700 CG PHE 292 12.003 12.113 62.167 1.00 16.59
ATOM 701 CD1 PHE 292 11.588 10.812 62.389 1.00 18.96
ATOM 702 CD2 PHE 292 12.002 12.607 60.875 1.00 19.01
ATOM 703 CE1 PHE 292 11.170 10.011 61.332 1.00 20.62
ATOM 704 CE2 PHE 292 11.581 11.805 59.805 1.00 18.46
ATOM 705 CZ PHE 292 11.166 10.499 60.060 1.00 18.06
ATOM 706 C PHE 292 14.761 12.191 63.713 1.00 15.70
ATOM 707 O PHE 292 15.132 11.119 63.236 1.00 15.72
ATOM 708 N ALA 293 15.526 13.278 63.760 1.00 16.34
ATOM 709 CA ALA 293 16.906 13.267 63.232 1.00 16.73
ATOM 710 CB ALA 293 17.464 14.702 63.207 1.00 17.74

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ATOM   711  C   ALA  293     17.802  12.368  64.090  1.00 17.09
ATOM   712  O   ALA  293     18.668  11.654  63.570  1.00 17.27
ATOM   713  N   ILE  294     17.623  12.423  65.407  1.00 16.09
ATOM   714  CA  ILE  294     18.389  11.569  66.312  1.00 16.22
ATOM   715  CB  ILE  294     18.032  11.857  67.768  1.00 15.67
ATOM   716  CG2 ILE  294     18.584  10.765  68.679  1.00 16.66
ATOM   717  CG1 ILE  294     18.615  13.218  68.160  1.00 17.00
ATOM   718  CD1 ILE  294     18.206  13.635  69.535  1.00 20.77
ATOM   719  C   ILE  294     18.070  10.111  65.971  1.00 16.74
ATOM   720  O   ILE  294     18.954   9.296  65.833  1.00 16.38
ATOM   721  N   ALA  295     16.791   9.791  65.774  1.00 16.15
ATOM   722  CA  ALA  295     16.452   8.420  65.424  1.00 16.99
ATOM   723  CB  ALA  295     14.937   8.273  65.332  1.00 16.54
ATOM   724  C   ALA  295     17.083   7.993  64.088  1.00 17.97
ATOM   725  O   ALA  295     17.563   6.870  63.954  1.00 18.01
ATOM   726  N   TRP  296     17.071   8.881  63.102  1.00 18.59
ATOM   727  CA  TRP  296     17.625   8.570  61.782  1.00 18.81
ATOM   728  CB  TRP  296     17.321   9.740  60.835  1.00 20.21
ATOM   729  CG  TRP  296     17.849   9.622  59.451  1.00 22.61
ATOM   730  CD2 TRP  296     17.398   8.716  58.433  1.00 25.62
ATOM   731  CE2 TRP  296     18.125   9.007  57.265  1.00 26.25
ATOM   732  CE3 TRP  296     16.448   7.683  58.402  1.00 25.95
ATOM   733  CD1 TRP  296     18.807  10.403  58.871  1.00 26.23
ATOM   734  NE1 TRP  296     18.975  10.043  57.556  1.00 26.50
ATOM   735  CZ2 TRP  296     17.934   8.297  56.063  1.00 27.77
ATOM   736  CZ3 TRP  296     16.257   6.977  57.206  1.00 27.65
ATOM   737  CH2 TRP  296     16.996   7.289  56.061  1.00 25.35
ATOM   738  C   TRP  296     19.133   8.299  61.878  1.00 19.53
ATOM   739  O   TRP  296     19.647   7.296  61.345  1.00 21.43
ATOM   740  N   ARG  297     19.833   9.147  62.623  1.00 18.58
ATOM   741  CA  ARG  297     21.280   8.974  62.748  1.00 18.22
ATOM   742  CB  ARG  297     21.923  10.208  63.376  1.00 18.92
ATOM   743  CG  ARG  297     21.886  11.465  62.525  1.00 20.63
ATOM   744  CD  ARG  297     22.792  12.530  63.137  1.00 26.15
ATOM   745  NE  ARG  297     22.219  13.002  64.381  1.00 29.32
ATOM   746  CZ  ARG  297     21.393  14.040  64.462  1.00 28.97
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ATOM	747	NH1	ARG	297	21.066	14.720	63.373	1.00	29.81
ATOM	748	NH2	ARG	297	20.872	14.372	65.628	1.00	31.03
ATOM	749	C	ARG	297	21.643	7.776	63.605	1.00	18.87
ATOM	750	O	ARG	297	22.738	7.225	63.473	1.00	19.01
ATOM	751	N	SER	298	20.749	7.404	64.511	1.00	17.52
ATOM	752	CA	SER	298	21.023	6.293	65.414	1.00	18.09
ATOM	753	CB	SER	298	20.134	6.407	66.655	1.00	18.94
ATOM	754	OG	SER	298	20.412	7.606	67.381	1.00	18.16
ATOM	755	C	SER	298	20.865	4.929	64.770	1.00	20.63
ATOM	756	O	SER	298	21.310	3.925	65.336	1.00	24.22
ATOM	757	N	MET	299	20.270	4.868	63.582	1.00	20.01
ATOM	758	CA	MET	299	20.106	3.558	62.953	1.00	22.16
ATOM	759	CB	MET	299	19.367	3.682	61.610	1.00	24.42
ATOM	760	CG	MET	299	17.940	4.159	61.735	1.00	24.29
ATOM	761	SD	MET	299	17.091	4.052	60.130	1.00	31.30
ATOM	762	CE	MET	299	18.221	4.950	59.082	1.00	31.06
ATOM	763	C	MET	299	21.431	2.825	62.725	1.00	25.30
ATOM	764	O	MET	299	21.493	1.600	62.859	1.00	26.84
ATOM	765	N	GLU	300	22.485	3.565	62.414	1.00	28.43
ATOM	766	CA	GLU	300	23.775	2.944	62.117	1.00	32.11
ATOM	767	CB	GLU	300	24.736	3.949	61.472	1.00	34.60
ATOM	768	CG	GLU	300	25.355	4.941	62.420	1.00	40.06
ATOM	769	CD	GLU	300	26.689	5.477	61.910	1.00	43.56
ATOM	770	OE1	GLU	300	27.622	4.666	61.729	1.00	46.83
ATOM	771	OE2	GLU	300	26.812	6.703	61.688	1.00	45.34
ATOM	772	C	GLU	300	24.467	2.304	63.300	1.00	32.94
ATOM	773	O	GLU	300	25.389	1.517	63.123	1.00	32.67
ATOM	774	N	PHE	301	24.033	2.649	64.507	1.00	31.51
ATOM	775	CA	PHE	301	24.632	2.094	65.710	1.00	32.60
ATOM	776	CB	PHE	301	24.822	3.214	66.736	1.00	32.49
ATOM	777	CG	PHE	301	25.879	4.203	66.349	1.00	34.07
ATOM	778	CD1	PHE	301	27.223	3.838	66.358	1.00	33.32
ATOM	779	CD2	PHE	301	25.537	5.483	65.929	1.00	33.10
ATOM	780	CE1	PHE	301	28.207	4.737	65.949	1.00	34.17
ATOM	781	CE2	PHE	301	26.506	6.385	65.519	1.00	34.69
ATOM	782	CZ	PHE	301	27.854	6.008	65.530	1.00	33.21

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ATOM   783  C   PHE  301     23.820   0.940  66.301  1.00 33.77
ATOM   784  O   PHE  301     24.127   0.441  67.377  1.00 34.55
ATOM   785  N   LEU  302     22.780   0.516  65.589  1.00 34.80
ATOM   786  CA  LEU  302     21.966  -0.593  66.045  1.00 36.81
ATOM   787  CB  LEU  302     20.641  -0.645  65.287  1.00 34.98
ATOM   788  CG  LEU  302     19.779   0.596  65.488  1.00 31.61
ATOM   789  CD1 LEU  302     18.551   0.528  64.577  1.00 31.62
ATOM   790  CD2 LEU  302     19.386   0.717  66.955  1.00 31.48
ATOM   791  C   LEU  302     22.744  -1.869  65.775  1.00 40.52
ATOM   792  O   LEU  302     23.333  -2.038  64.701  1.00 40.16
ATOM   793  N   THR  303     22.733  -2.764  66.753  1.00 44.10
ATOM   794  CA  THR  303     23.422  -4.037  66.634  1.00 48.80
ATOM   795  CB  THR  303     23.126  -4.933  67.850  1.00 49.83
ATOM   796  OG1 THR  303     23.211  -4.151  69.050  1.00 51.18
ATOM   797  CG2 THR  303     24.132  -6.076  67.924  1.00 51.25
ATOM   798  C   THR  303     22.932  -4.731  65.368  1.00 50.84
ATOM   799  O   THR  303     21.739  -4.703  65.052  1.00 50.20
ATOM   800  N   ALA  304     23.864  -5.341  64.644  1.00 53.24
ATOM   801  CA  ALA  304     23.538  -6.040  63.410  1.00 55.88
ATOM   802  CB  ALA  304     24.739  -6.867  62.946  1.00 56.05
ATOM   803  C   ALA  304     22.317  -6.942  63.575  1.00 57.61
ATOM   804  O   ALA  304     22.133  -7.583  64.617  1.00 58.45
ATOM   805  N   ALA  305     21.481  -6.972  62.540  1.00 59.51
ATOM   806  CA  ALA  305     20.282  -7.797  62.535  1.00 60.68
ATOM   807  CB  ALA  305     19.548  -7.651  61.205  1.00 60.98
ATOM   808  C   ALA  305     20.714  -9.245  62.744  1.00 61.71
ATOM   809  O   ALA  305     19.925 -10.029  63.319  1.00 62.15
ATOM   810  OXT ALA  305     21.848  -9.572  62.316  1.00 61.88
ATOM   811  CB  ALA  316     17.484 -11.402  70.435  1.00 59.02
ATOM   812  C   ALA  316     15.833  -9.781  71.403  1.00 57.95
ATOM   813  O   ALA  316     15.469  -9.327  70.316  1.00 58.69
ATOM   814  N   ALA  316     15.341 -12.224  71.375  1.00 58.18
ATOM   815  CA  ALA  316     16.413 -11.191  71.510  1.00 58.61
ATOM   816  N   ALA  317     15.747  -9.096  72.539  1.00 56.79
ATOM   817  CA  ALA  317     15.218  -7.739  72.587  1.00 54.70
ATOM   818  CB  ALA  317     13.813  -7.745  73.174  1.00 54.73
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ATOM   819  C   ALA  317     16.142  -6.871  73.437  1.00 52.91
ATOM   820  O   ALA  317     15.697  -5.935  74.111  1.00 53.06
ATOM   821  N   SER  318     17.430  -7.207  73.404  1.00 49.42
ATOM   822  CA  SER  318     18.449  -6.478  74.151  1.00 46.14
ATOM   823  CB  SER  318     19.830  -7.056  73.835  1.00 46.72
ATOM   824  OG  SER  318     20.834  -6.462  74.639  1.00 47.98
ATOM   825  C   SER  318     18.378  -5.009  73.723  1.00 43.02
ATOM   826  O   SER  318     18.543  -4.686  72.541  1.00 44.27
ATOM   827  N   PRO  319     18.122  -4.100  74.676  0.50 41.03      AC1
ATOM   828  CD  PRO  319     17.740  -4.342  76.079  0.50 40.29      AC1
ATOM   829  CA  PRO  319     18.033  -2.672  74.351  0.50 38.31      AC1
ATOM   830  CB  PRO  319     17.690  -2.032  75.694  0.50 38.96      AC1
ATOM   831  CG  PRO  319     16.927  -3.116  76.402  0.50 39.34      AC1
ATOM   832  C   PRO  319     19.310  -2.080  73.756  0.50 35.85      AC1
ATOM   833  O   PRO  319     20.394  -2.240  74.319  0.50 35.73      AC1
ATOM   834  N   PRO  320     19.197  -1.403  72.599  1.00 33.69
ATOM   835  CD  PRO  320     18.041  -1.404  71.692  1.00 32.09
ATOM   836  CA  PRO  320     20.362  -0.784  71.952  1.00 30.83
ATOM   837  CB  PRO  320     19.769  -0.083  70.722  1.00 30.11
ATOM   838  CG  PRO  320     18.279  -0.174  70.892  1.00 32.74
ATOM   839  C   PRO  320     21.008   0.185  72.949  1.00 27.19
ATOM   840  O   PRO  320     20.317   0.824  73.756  1.00 27.36
ATOM   841  N   GLN  321     22.328   0.297  72.890  1.00 25.76
ATOM   842  CA  GLN  321     23.060   1.121  73.847  1.00 25.85
ATOM   843  CB  GLN  321     24.262   0.329  74.357  1.00 29.20
ATOM   844  CG  GLN  321     23.925  -1.090  74.757  1.00 34.12
ATOM   845  CD  GLN  321     23.408  -1.197  76.163  1.00 38.11
ATOM   846  OE1 GLN  321     24.127  -0.916  77.123  1.00 40.85
ATOM   847  NE2 GLN  321     22.150  -1.617  76.302  1.00 40.57
ATOM   848  C   GLN  321     23.546   2.495  73.423  1.00 23.90
ATOM   849  O   GLN  321     23.914   3.297  74.275  1.00 24.18
ATOM   850  N   LEU  322     23.536   2.790  72.128  1.00 22.59
ATOM   851  CA  LEU  322     24.050   4.080  71.666  1.00 21.41
ATOM   852  CB  LEU  322     25.291   3.879  70.775  1.00 22.86
ATOM   853  CG  LEU  322     26.560   3.362  71.432  1.00 25.45
ATOM   854  CD1 LEU  322     27.625   3.130  70.345  1.00 28.06
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ATOM   855 CD2 LEU  322     27.036   4.384  72.497  1.00 24.21
ATOM   856 C   LEU  322     23.079   4.942  70.891  1.00 22.08
ATOM   857 O   LEU  322     22.435   4.478  69.961  1.00 23.11
ATOM   858 N   MET  323     23.003   6.205  71.270  1.00 20.81
ATOM   859 CA  MET  323     22.145   7.157  70.590  1.00 21.91
ATOM   860 CB  MET  323     21.213   7.835  71.598  1.00 23.20
ATOM   861 CG  MET  323     20.325   8.922  70.978  1.00 22.36
ATOM   862 SD  MET  323     19.196   9.636  72.187  1.00 22.04
ATOM   863 CE  MET  323     18.026   8.314  72.302  1.00 22.12
ATOM   864 C   MET  323     23.054   8.187  69.914  1.00 25.54
ATOM   865 O   MET  323     24.002   8.691  70.530  1.00 25.31
ATOM   866 N   CYS  324     22.781   8.506  68.650  1.00 22.41
ATOM   867 CA  CYS  324     23.619   9.483  67.941  1.00 24.83
ATOM   868 CB  CYS  324     23.854   9.029  66.512  1.00 23.91
ATOM   869 SG  CYS  324     24.921  10.185  65.588  1.00 27.74
ATOM   870 C   CYS  324     22.995  10.873  67.950  1.00 24.34
ATOM   871 O   CYS  324     22.010  11.148  67.249  1.00 24.90
ATOM   872 N   LEU  325     23.560  11.758  68.749  1.00 24.49
ATOM   873 CA  LEU  325     23.038  13.114  68.843  1.00 25.66
ATOM   874 CB  LEU  325     23.421  13.746  70.183  1.00 26.79
ATOM   875 CG  LEU  325     22.935  12.964  71.421  1.00 27.19
ATOM   876 CD1 LEU  325     23.256  13.744  72.704  1.00 29.28
ATOM   877 CD2 LEU  325     21.423  12.732  71.320  1.00 27.92
ATOM   878 C   LEU  325     23.513  13.990  67.682  1.00 28.10
ATOM   879 O   LEU  325     22.860  14.978  67.344  1.00 31.20
ATOM   880 N   MET  326     24.650  13.618  67.094  1.00 28.83
ATOM   881 CA  MET  326     25.253  14.311  65.947  1.00 30.95
ATOM   882 CB  MET  326     25.726  15.721  66.350  1.00 31.86
ATOM   883 CG  MET  326     26.894  15.710  67.335  1.00 31.84
ATOM   884 SD  MET  326     27.648  17.333  67.693  1.00 34.98
ATOM   885 CE  MET  326     29.085  16.800  68.706  1.00 30.77
ATOM   886 C   MET  326     26.462  13.453  65.513  1.00 33.06
ATOM   887 O   MET  326     26.882  12.565  66.242  1.00 32.71
ATOM   888 N   PRO  327     27.013  13.682  64.307  1.00 35.54
ATOM   889 CD  PRO  327     26.511  14.545  63.227  1.00 35.87
ATOM   890 CA  PRO  327     28.180  12.896  63.857  1.00 36.24
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ATOM	891	CB	PRO	327	28.508	13.519	62.503	1.00	37.87
ATOM	892	CG	PRO	327	27.159	13.932	62.001	1.00	35.11
ATOM	893	C	PRO	327	29.353	13.035	64.836	1.00	38.75
ATOM	894	O	PRO	327	29.754	14.154	65.155	1.00	38.99
ATOM	895	N	GLY	328	29.890	11.908	65.314	1.00	38.52
ATOM	896	CA	GLY	328	31.001	11.933	66.257	1.00	38.65
ATOM	897	C	GLY	328	30.606	12.217	67.700	1.00	38.39
ATOM	898	O	GLY	328	31.431	12.604	68.545	1.00	39.05
ATOM	899	N	MET	329	29.326	12.020	67.994	1.00	36.32
ATOM	900	CA	MET	329	28.830	12.251	69.326	1.00	34.24
ATOM	901	CB	MET	329	28.343	13.693	69.451	1.00	38.91
ATOM	902	CG	MET	329	27.462	13.991	70.649	1.00	44.24
ATOM	903	SD	MET	329	28.233	13.696	72.235	1.00	50.95
ATOM	904	CE	MET	329	26.854	12.835	73.089	1.00	48.58
ATOM	905	C	MET	329	27.700	11.271	69.603	1.00	30.52
ATOM	906	O	MET	329	26.647	11.331	68.975	1.00	28.92
ATOM	907	N	THR	330	27.960	10.324	70.490	1.00	26.42
ATOM	908	CA	THR	330	26.933	9.370	70.865	1.00	23.65
ATOM	909	CB	THR	330	27.338	7.895	70.542	1.00	24.12
ATOM	910	OG1	THR	330	28.672	7.654	71.005	1.00	27.18
ATOM	911	CG2	THR	330	27.269	7.622	69.034	1.00	26.34
ATOM	912	C	THR	330	26.685	9.475	72.360	1.00	23.23
ATOM	913	O	THR	330	27.572	9.802	73.146	1.00	23.91
ATOM	914	N	LEU	331	25.450	9.211	72.748	1.00	20.37
ATOM	915	CA	LEU	331	25.082	9.213	74.142	1.00	21.33
ATOM	916	CB	LEU	331	23.773	9.986	74.340	1.00	24.38
ATOM	917	CG	LEU	331	23.113	9.731	75.696	1.00	25.70
ATOM	918	CD1	LEU	331	23.979	10.317	76.825	1.00	30.48
ATOM	919	CD2	LEU	331	21.723	10.348	75.694	1.00	29.64
ATOM	920	C	LEU	331	24.892	7.737	74.489	1.00	21.13
ATOM	921	O	LEU	331	24.158	7.026	73.819	1.00	19.21
ATOM	922	N	HIS	332	25.582	7.262	75.525	1.00	18.80
ATOM	923	CA	HIS	332	25.472	5.864	75.901	1.00	18.64
ATOM	924	CB	HIS	332	26.740	5.417	76.658	1.00	18.77
ATOM	925	CG	HIS	332	26.826	3.938	76.862	1.00	21.68
ATOM	926	CD2	HIS	332	27.533	2.991	76.205	1.00	22.97

ATOM	927	ND1	HIS	332	26.092	3.273	77.824	1.00	22.38
ATOM	928	CE1	HIS	332	26.340	1.978	77.745	1.00	23.74
ATOM	929	NE2	HIS	332	27.213	1.778	76.769	1.00	25.26
ATOM	930	C	HIS	332	24.262	5.721	76.820	1.00	18.95
ATOM	931	O	HIS	332	23.981	6.620	77.616	1.00	19.91
ATOM	932	N	ARG	333	23.594	4.581	76.715	1.00	19.39
ATOM	933	CA	ARG	333	22.394	4.282	77.509	1.00	19.71
ATOM	934	CB	ARG	333	21.930	2.850	77.235	1.00	20.65
ATOM	935	CG	ARG	333	20.582	2.512	77.896	1.00	21.54
ATOM	936	CD	ARG	333	20.018	1.212	77.353	1.00	21.69
ATOM	937	NE	ARG	333	18.703	0.862	77.899	1.00	20.98
ATOM	938	CZ	ARG	333	18.501	0.034	78.921	1.00	22.46
ATOM	939	NH1	ARG	333	19.535	-0.547	79.531	1.00	24.12
ATOM	940	NH2	ARG	333	17.255	-0.241	79.309	1.00	20.87
ATOM	941	C	ARG	333	22.643	4.463	79.018	1.00	21.14
ATOM	942	O	ARG	333	21.782	4.926	79.755	1.00	18.39
ATOM	943	N	ASN	334	23.832	4.107	79.484	1.00	21.27
ATOM	944	CA	ASN	334	24.114	4.259	80.910	1.00	23.47
ATOM	945	CB	ASN	334	25.486	3.653	81.244	1.00	24.93
ATOM	946	CG	ASN	334	25.504	2.119	81.158	1.00	25.59
ATOM	947	OD1	ASN	334	24.467	1.461	81.054	1.00	26.24
ATOM	948	ND2	ASN	334	26.707	1.544	81.204	1.00	29.08
ATOM	949	C	ASN	334	24.048	5.718	81.380	1.00	22.91
ATOM	950	O	ASN	334	23.649	6.000	82.530	1.00	22.99
ATOM	951	N	SER	335	24.441	6.657	80.524	1.00	22.89
ATOM	952	CA	SER	335	24.378	8.059	80.904	1.00	22.41
ATOM	953	CB	SER	335	25.178	8.915	79.930	1.00	27.35
ATOM	954	OG	SER	335	26.517	8.437	79.856	1.00	31.39
ATOM	955	C	SER	335	22.908	8.484	80.939	1.00	23.03
ATOM	956	O	SER	335	22.496	9.260	81.809	1.00	22.21
ATOM	957	N	ALA	336	22.126	7.970	79.989	1.00	21.81
ATOM	958	CA	ALA	336	20.703	8.255	79.952	1.00	21.09
ATOM	959	CB	ALA	336	20.060	7.595	78.718	1.00	21.81
ATOM	960	C	ALA	336	20.044	7.744	81.232	1.00	21.37
ATOM	961	O	ALA	336	19.209	8.425	81.830	1.00	19.40
ATOM	962	N	LEU	337	20.423	6.540	81.660	1.00	19.77

ATOM	963	CA	LEU	337	19.860	5.960	82.865	1.00	19.59
ATOM	964	CB	LEU	337	20.374	4.517	83.039	1.00	19.20
ATOM	965	CG	LEU	337	19.835	3.502	82.031	1.00	20.97
ATOM	966	CD1	LEU	337	20.702	2.280	82.055	1.00	23.49
ATOM	967	CD2	LEU	337	18.391	3.164	82.329	1.00	21.07
ATOM	968	C	LEU	337	20.206	6.777	84.089	1.00	20.54
ATOM	969	O	LEU	337	19.364	6.997	84.985	1.00	19.57
ATOM	970	N	GLN	338	21.454	7.226	84.131	1.00	21.36
ATOM	971	CA	GLN	338	21.920	7.994	85.264	1.00	22.39
ATOM	972	CB	GLN	338	23.439	8.206	85.179	1.00	22.44
ATOM	973	CG	GLN	338	23.973	8.755	86.488	1.00	27.14
ATOM	974	CD	GLN	338	25.467	9.026	86.481	1.00	29.23
ATOM	975	OE1	GLN	338	25.955	9.827	87.278	1.00	30.73
ATOM	976	NE2	GLN	338	26.196	8.360	85.596	1.00	30.79
ATOM	977	C	GLN	338	21.200	9.331	85.381	1.00	23.40
ATOM	978	O	GLN	338	20.894	9.790	86.490	1.00	21.75
ATOM	979	N	ALA	339	20.899	9.935	84.227	1.00	22.63
ATOM	980	CA	ALA	339	20.215	11.217	84.191	1.00	24.41
ATOM	981	CB	ALA	339	20.430	11.903	82.832	1.00	23.46
ATOM	982	C	ALA	339	18.727	11.082	84.463	1.00	24.73
ATOM	983	O	ALA	339	18.059	12.084	84.641	1.00	27.16
ATOM	984	N	GLY	340	18.218	9.850	84.499	1.00	22.58
ATOM	985	CA	GLY	340	16.803	9.622	84.754	1.00	23.89
ATOM	986	C	GLY	340	15.898	9.580	83.531	1.00	25.09
ATOM	987	O	GLY	340	14.666	9.607	83.666	1.00	25.54
ATOM	988	N	VAL	341	16.492	9.479	82.346	1.00	23.51
ATOM	989	CA	VAL	341	15.719	9.473	81.095	1.00	20.92
ATOM	990	CB	VAL	341	16.134	10.677	80.211	1.00	21.83
ATOM	991	CG1	VAL	341	15.838	11.981	80.942	1.00	21.94
ATOM	992	CG2	VAL	341	17.621	10.577	79.858	1.00	21.91
ATOM	993	C	VAL	341	15.891	8.185	80.300	1.00	20.24
ATOM	994	O	VAL	341	15.803	8.182	79.083	1.00	19.53
ATOM	995	N	GLY	342	16.132	7.079	80.999	1.00	19.65
ATOM	996	CA	GLY	342	16.324	5.827	80.301	1.00	18.76
ATOM	997	C	GLY	342	15.104	5.352	79.541	1.00	19.27
ATOM	998	O	GLY	342	15.230	4.771	78.470	1.00	18.82

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ATOM   999 N   GLN  343    13.922  5.598 80.088 0.50 18.31    AC1
ATOM  1000 CA  GLN  343    12.706  5.163 79.422 0.50 19.11    AC1
ATOM  1001 CB  GLN  343    11.507  5.485 80.305 0.50 19.94    AC1
ATOM  1002 CG  GLN  343    10.200  4.866 79.867 0.50 22.91    AC1
ATOM  1003 CD  GLN  343     9.082  5.177 80.852 0.50 24.13    AC1
ATOM  1004 OE1 GLN  343     8.669  6.326 80.995 0.50 26.85    AC1
ATOM  1005 NE2 GLN  343     8.606  4.154 81.555 0.50 25.40    AC1
ATOM  1006 C   GLN  343    12.542  5.813 78.043 0.50 19.14    AC1
ATOM  1007 O   GLN  343    12.318  5.127 77.050 0.50 18.83    AC1
ATOM  1008 N   ILE  344    12.664  7.136 77.977 1.00 17.95
ATOM  1009 CA  ILE  344    12.506  7.812 76.693 1.00 17.74
ATOM  1010 CB  ILE  344    12.348  9.372 76.875 1.00 18.47
ATOM  1011 CG2 ILE  344    13.700 10.010 77.231 1.00 20.66
ATOM  1012 CG1 ILE  344    11.754  9.984 75.596 1.00 19.04
ATOM  1013 CD1 ILE  344    11.445 11.499 75.662 1.00 21.07
ATOM  1014 C   ILE  344    13.641  7.448 75.718 1.00 17.34
ATOM  1015 O   ILE  344    13.440  7.389 74.499 1.00 16.12
ATOM  1016 N   PHE  345    14.844  7.210 76.248 1.00 16.60
ATOM  1017 CA  PHE  345    15.976  6.826 75.417 1.00 17.63
ATOM  1018 CB  PHE  345    17.208  6.636 76.322 1.00 17.86
ATOM  1019 CG  PHE  345    18.455  6.189 75.613 1.00 18.24
ATOM  1020 CD1 PHE  345    18.657  4.848 75.273 1.00 18.20
ATOM  1021 CD2 PHE  345    19.470  7.090 75.363 1.00 20.10
ATOM  1022 CE1 PHE  345    19.854  4.412 74.706 1.00 19.01
ATOM  1023 CE2 PHE  345    20.663  6.673 74.798 1.00 17.96
ATOM  1024 CZ  PHE  345    20.861  5.328 74.469 1.00 18.58
ATOM  1025 C   PHE  345    15.603  5.522 74.710 1.00 18.98
ATOM  1026 O   PHE  345    15.756  5.389 73.491 1.00 18.15
ATOM  1027 N   ASP  346    15.072  4.568 75.480 1.00 18.04
ATOM  1028 CA  ASP  346    14.695  3.300 74.894 1.00 18.83
ATOM  1029 CB  ASP  346    14.285  2.302 75.988 1.00 19.96
ATOM  1030 CG  ASP  346    15.467  1.768 76.786 1.00 24.04
ATOM  1031 OD1 ASP  346    16.630  2.038 76.430 1.00 24.95
ATOM  1032 OD2 ASP  346    15.232  1.043 77.784 1.00 24.86
ATOM  1033 C   ASP  346    13.550  3.462 73.872 1.00 18.04
ATOM  1034 O   ASP  346    13.549  2.782 72.841 1.00 19.39
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ATOM 1035 N ARG 347 12.603 4.359 74.138 1.00 19.77
ATOM 1036 CA ARG 347 11.493 4.579 73.188 1.00 20.42
ATOM 1037 CB ARG 347 10.443 5.558 73.708 1.00 24.20
ATOM 1038 CG ARG 347 9.527 5.024 74.786 1.00 26.30
ATOM 1039 CD ARG 347 8.310 5.929 74.937 1.00 28.76
ATOM 1040 NE ARG 347 7.383 5.807 73.813 1.00 29.58
ATOM 1041 CZ ARG 347 6.312 6.577 73.629 1.00 31.91
ATOM 1042 NH1 ARG 347 6.028 7.536 74.492 1.00 32.14
ATOM 1043 NH2 ARG 347 5.522 6.378 72.579 1.00 32.47
ATOM 1044 C ARG 347 12.012 5.120 71.875 1.00 20.09
ATOM 1045 O ARG 347 11.586 4.703 70.806 1.00 18.14
ATOM 1046 N VAL 348 12.939 6.073 71.945 1.00 18.48
ATOM 1047 CA VAL 348 13.480 6.621 70.708 1.00 18.94
ATOM 1048 CB VAL 348 14.532 7.713 70.991 1.00 18.19
ATOM 1049 CG1 VAL 348 15.286 8.052 69.706 1.00 18.18
ATOM 1050 CG2 VAL 348 13.862 8.930 71.600 1.00 19.11
ATOM 1051 C VAL 348 14.143 5.518 69.882 1.00 18.63
ATOM 1052 O VAL 348 13.885 5.380 68.691 1.00 17.99
ATOM 1053 N LEU 349 14.981 4.709 70.514 1.00 18.35
ATOM 1054 CA LEU 349 15.679 3.686 69.749 1.00 19.38
ATOM 1055 CB LEU 349 16.906 3.175 70.526 1.00 20.34
ATOM 1056 CG LEU 349 17.920 4.286 70.807 1.00 20.49
ATOM 1057 CD1 LEU 349 19.173 3.626 71.408 1.00 23.32
ATOM 1058 CD2 LEU 349 18.273 5.078 69.500 1.00 18.92
ATOM 1059 C LEU 349 14.822 2.509 69.294 1.00 20.39
ATOM 1060 O LEU 349 15.112 1.901 68.263 1.00 19.62
ATOM 1061 N SER 350 13.746 2.208 70.025 1.00 21.15
ATOM 1062 CA SER 350 12.907 1.074 69.623 1.00 23.27
ATOM 1063 CB SER 350 12.443 0.294 70.855 1.00 25.65
ATOM 1064 OG SER 350 11.622 1.081 71.687 1.00 28.64
ATOM 1065 C SER 350 11.698 1.451 68.766 1.00 21.84
ATOM 1066 O SER 350 11.424 0.790 67.762 1.00 25.35
ATOM 1067 N GLU 351 10.986 2.516 69.131 1.00 22.62
ATOM 1068 CA GLU 351 9.801 2.906 68.368 1.00 22.04
ATOM 1069 CB GLU 351 8.834 3.680 69.252 1.00 22.43
ATOM 1070 CG GLU 351 8.454 2.916 70.486 1.00 26.86

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ATOM  1071  CD  GLU  351      7.434   3.650  71.303  1.00 28.97
ATOM  1072  OE1 GLU  351      7.473   3.544  72.548  1.00 31.85
ATOM  1073  OE2 GLU  351      6.581   4.330  70.691  1.00 32.68
ATOM  1074  C   GLU  351     10.133   3.708  67.132  1.00 22.11
ATOM  1075  O   GLU  351      9.348   3.766  66.183  1.00 22.30
ATOM  1076  N   LEU  352     11.309   4.328  67.113  1.00 19.99
ATOM  1077  CA  LEU  352     11.696   5.083  65.934  1.00 19.01
ATOM  1078  CB  LEU  352     12.043   6.555  66.293  1.00 18.64
ATOM  1079  CG  LEU  352     10.911   7.365  66.950  1.00 19.12
ATOM  1080  CD1 LEU  352     11.445   8.742  67.339  1.00 19.51
ATOM  1081  CD2 LEU  352      9.703   7.505  66.018  1.00 19.25
ATOM  1082  C   LEU  352     12.859   4.467  65.163  1.00 19.51
ATOM  1083  O   LEU  352     12.704   3.977  64.038  1.00 21.10
ATOM  1084  N   SER  353     14.052   4.464  65.754  0.50 18.72    AC1
ATOM  1085  CA  SER  353     15.203   3.933  65.034  0.50 18.55    AC1
ATOM  1086  CB  SER  353     16.473   4.032  65.883  0.50 16.66    AC1
ATOM  1087  OG  SER  353     16.782   5.378  66.160  0.50 11.47    AC1
ATOM  1088  C   SER  353     15.045   2.500  64.546  0.50 19.60    AC1
ATOM  1089  O   SER  353     15.207   2.236  63.355  0.50 20.26    AC1
ATOM  1090  N   LEU  354     14.746   1.579  65.455  1.00 21.67
ATOM  1091  CA  LEU  354     14.602   0.181  65.051  1.00 23.55
ATOM  1092  CB  LEU  354     14.360  -0.715  66.278  1.00 24.35
ATOM  1093  CG  LEU  354     14.284  -2.222  66.012  1.00 30.18
ATOM  1094  CD1 LEU  354     15.388  -2.664  65.055  1.00 31.88
ATOM  1095  CD2 LEU  354     14.392  -2.944  67.345  1.00 31.36
ATOM  1096  C   LEU  354     13.489  -0.011  64.009  1.00 24.82
ATOM  1097  O   LEU  354     13.696  -0.684  63.004  1.00 25.66
ATOM  1098  N   LYS  355     12.324   0.587  64.234  1.00 26.97
ATOM  1099  CA  LYS  355     11.236   0.454  63.272  1.00 26.95
ATOM  1100  CB  LYS  355     10.003   1.226  63.735  1.00 29.30
ATOM  1101  CG  LYS  355      9.228   0.572  64.843  1.00 34.34
ATOM  1102  CD  LYS  355      8.440  -0.616  64.321  1.00 38.57
ATOM  1103  CE  LYS  355      7.365  -1.007  65.319  1.00 39.54
ATOM  1104  NZ  LYS  355      7.883  -0.958  66.713  1.00 40.20
ATOM  1105  C   LYS  355     11.637   0.964  61.899  1.00 27.30
ATOM  1106  O   LYS  355     11.281   0.369  60.883  1.00 28.58
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ATOM	1107	N	MET	356	12.362	2.080	61.860	1.00	25.41
ATOM	1108	CA	MET	356	12.787	2.641	60.594	1.00	25.37
ATOM	1109	CB	MET	356	13.279	4.071	60.778	1.00	27.04
ATOM	1110	CG	MET	356	12.126	5.017	60.918	1.00	26.57
ATOM	1111	SD	MET	356	12.669	6.671	60.768	1.00	36.72
ATOM	1112	CE	MET	356	13.015	6.835	62.357	1.00	16.80
ATOM	1113	C	MET	356	13.836	1.808	59.896	1.00	26.93
ATOM	1114	O	MET	356	13.907	1.807	58.676	1.00	25.41
ATOM	1115	N	ARG	357	14.672	1.114	60.661	1.00	27.88
ATOM	1116	CA	ARG	357	15.656	0.281	60.003	1.00	29.75
ATOM	1117	CB	ARG	357	16.733	-0.214	60.961	1.00	31.09
ATOM	1118	CG	ARG	357	17.748	-1.056	60.213	1.00	35.17
ATOM	1119	CD	ARG	357	18.840	-1.607	61.112	1.00	38.46
ATOM	1120	NE	ARG	357	18.313	-2.543	62.097	1.00	41.53
ATOM	1121	CZ	ARG	357	19.066	-3.164	63.003	1.00	43.38
ATOM	1122	NH1	ARG	357	20.376	-2.942	63.037	1.00	42.92
ATOM	1123	NH2	ARG	357	18.512	-3.995	63.879	1.00	43.48
ATOM	1124	C	ARG	357	14.926	-0.925	59.422	1.00	29.63
ATOM	1125	O	ARG	357	15.218	-1.353	58.310	1.00	29.83
ATOM	1126	N	THR	358	13.966	-1.452	60.171	1.00	29.51
ATOM	1127	CA	THR	358	13.204	-2.609	59.704	1.00	30.65
ATOM	1128	CB	THR	358	12.273	-3.117	60.812	1.00	31.00
ATOM	1129	OG1	THR	358	13.071	-3.609	61.895	1.00	32.46
ATOM	1130	CG2	THR	358	11.374	-4.260	60.306	1.00	34.28
ATOM	1131	C	THR	358	12.408	-2.281	58.438	1.00	30.73
ATOM	1132	O	THR	358	12.286	-3.114	57.533	1.00	32.33
ATOM	1133	N	LEU	359	11.895	-1.056	58.359	1.00	29.40
ATOM	1134	CA	LEU	359	11.124	-0.610	57.201	1.00	29.68
ATOM	1135	CB	LEU	359	10.242	0.583	57.605	1.00	30.32
ATOM	1136	CG	LEU	359	8.732	0.609	57.321	1.00	34.26
ATOM	1137	CD1	LEU	359	8.197	2.038	57.529	1.00	33.77
ATOM	1138	CD2	LEU	359	8.452	0.142	55.900	1.00	34.08
ATOM	1139	C	LEU	359	12.046	-0.168	56.066	1.00	28.77
ATOM	1140	O	LEU	359	11.585	0.164	54.974	1.00	27.98
ATOM	1141	N	ARG	360	13.349	-0.130	56.327	1.00	30.53
ATOM	1142	CA	ARG	360	14.315	0.310	55.327	1.00	30.15

ATOM 1143 CB ARG 360 14.381 -0.695 54.178 1.00 33.80
ATOM 1144 CG ARG 360 14.798 -2.076 54.625 1.00 36.43
ATOM 1145 CD ARG 360 14.018 -3.165 53.900 1.00 39.56
ATOM 1146 NE ARG 360 12.588 -3.168 54.226 1.00 41.14
ATOM 1147 CZ ARG 360 11.618 -2.942 53.340 1.00 42.18
ATOM 1148 NH1 ARG 360 11.918 -2.688 52.071 1.00 41.02
ATOM 1149 NH2 ARG 360 10.345 -2.983 53.717 1.00 42.86
ATOM 1150 C ARG 360 13.975 1.699 54.787 1.00 29.92
ATOM 1151 O ARG 360 14.073 1.958 53.592 1.00 28.84
ATOM 1152 N VAL 361 13.569 2.600 55.677 1.00 27.64
ATOM 1153 CA VAL 361 13.261 3.956 55.267 1.00 25.17
ATOM 1154 CB VAL 361 12.909 4.819 56.480 1.00 24.00
ATOM 1155 CG1 VAL 361 12.684 6.254 56.066 1.00 24.37
ATOM 1156 CG2 VAL 361 11.688 4.249 57.166 1.00 23.19
ATOM 1157 C VAL 361 14.504 4.525 54.594 1.00 25.34
ATOM 1158 O VAL 361 15.613 4.407 55.133 1.00 25.79
ATOM 1159 N ASP 362 14.344 5.109 53.404 1.00 24.62
ATOM 1160 CA ASP 362 15.481 5.712 52.718 1.00 24.80
ATOM 1161 CB ASP 362 15.540 5.316 51.223 1.00 27.01
ATOM 1162 CG ASP 362 14.307 5.720 50.433 1.00 29.25
ATOM 1163 OD1 ASP 362 13.697 6.764 50.731 1.00 27.58
ATOM 1164 OD2 ASP 362 13.963 4.987 49.479 1.00 32.41
ATOM 1165 C ASP 362 15.520 7.226 52.863 1.00 25.99
ATOM 1166 O ASP 362 14.631 7.823 53.486 1.00 25.65
ATOM 1167 N GLN 363 16.561 7.845 52.312 1.00 24.73
ATOM 1168 CA GLN 363 16.742 9.286 52.405 1.00 26.50
ATOM 1169 CB GLN 363 18.044 9.682 51.690 1.00 31.84
ATOM 1170 CG GLN 363 18.339 11.179 51.662 1.00 36.89
ATOM 1171 CD GLN 363 19.008 11.689 52.921 1.00 40.13
ATOM 1172 OE1 GLN 363 18.615 11.346 54.047 1.00 42.87
ATOM 1173 NE2 GLN 363 20.013 12.536 52.743 1.00 40.44
ATOM 1174 C GLN 363 15.540 10.070 51.855 1.00 25.17
ATOM 1175 O GLN 363 15.077 11.020 52.480 1.00 22.69
ATOM 1176 N ALA 364 15.023 9.659 50.701 1.00 24.53
ATOM 1177 CA ALA 364 13.863 10.340 50.099 1.00 22.80
ATOM 1178 CB ALA 364 13.524 9.691 48.753 1.00 22.91

ATOM	1179	C	ALA	364	12.631	10.326	51.022	1.00	21.81
ATOM	1180	O	ALA	364	11.946	11.336	51.178	1.00	21.88
ATOM	1181	N	GLU	365	12.362	9.188	51.636	1.00	22.72
ATOM	1182	CA	GLU	365	11.218	9.062	52.532	1.00	21.63
ATOM	1183	CB	GLU	365	10.990	7.585	52.856	1.00	22.68
ATOM	1184	CG	GLU	365	10.724	6.806	51.583	1.00	23.15
ATOM	1185	CD	GLU	365	10.797	5.303	51.723	1.00	28.04
ATOM	1186	OE1	GLU	365	11.632	4.813	52.501	1.00	26.39
ATOM	1187	OE2	GLU	365	10.034	4.607	51.010	1.00	27.63
ATOM	1188	C	GLU	365	11.454	9.881	53.798	1.00	22.43
ATOM	1189	O	GLU	365	10.557	10.570	54.298	1.00	22.18
ATOM	1190	N	TYR	366	12.681	9.822	54.304	1.00	22.10
ATOM	1191	CA	TYR	366	13.026	10.580	55.506	1.00	22.15
ATOM	1192	CB	TYR	366	14.494	10.316	55.871	1.00	22.04
ATOM	1193	CG	TYR	366	15.010	11.209	56.986	1.00	22.63
ATOM	1194	CD1	TYR	366	14.580	11.030	58.307	1.00	21.87
ATOM	1195	CE1	TYR	366	15.023	11.864	59.328	1.00	22.24
ATOM	1196	CD2	TYR	366	15.903	12.246	56.715	1.00	20.88
ATOM	1197	CE2	TYR	366	16.366	13.092	57.731	1.00	22.98
ATOM	1198	CZ	TYR	366	15.913	12.899	59.041	1.00	22.25
ATOM	1199	OH	TYR	366	16.315	13.752	60.054	1.00	23.04
ATOM	1200	C	TYR	366	12.797	12.095	55.332	1.00	19.98
ATOM	1201	O	TYR	366	12.209	12.731	56.199	1.00	19.55
ATOM	1202	N	VAL	367	13.260	12.676	54.225	1.00	20.09
ATOM	1203	CA	VAL	367	13.080	14.106	54.034	1.00	19.12
ATOM	1204	CB	VAL	367	13.955	14.666	52.891	1.00	20.38
ATOM	1205	CG1	VAL	367	15.446	14.473	53.249	1.00	21.37
ATOM	1206	CG2	VAL	367	13.609	14.009	51.554	1.00	19.90
ATOM	1207	C	VAL	367	11.607	14.458	53.784	1.00	18.65
ATOM	1208	O	VAL	367	11.165	15.538	54.178	1.00	18.48
ATOM	1209	N	ALA	368	10.868	13.552	53.147	1.00	20.47
ATOM	1210	CA	ALA	368	9.447	13.787	52.893	1.00	19.05
ATOM	1211	CB	ALA	368	8.854	12.668	51.988	1.00	18.93
ATOM	1212	C	ALA	368	8.714	13.813	54.240	1.00	19.17
ATOM	1213	O	ALA	368	7.863	14.682	54.487	1.00	18.81
ATOM	1214	N	LEU	369	9.048	12.871	55.112	1.00	19.43

ATOM	1215	CA	LEU	369	8.417	12.819	56.428	1.00	17.85
ATOM	1216	CB	LEU	369	8.807	11.526	57.147	1.00	20.14
ATOM	1217	CG	LEU	369	8.153	10.250	56.565	1.00	21.25
ATOM	1218	CD1	LEU	369	8.810	9.041	57.154	1.00	22.02
ATOM	1219	CD2	LEU	369	6.626	10.219	56.856	1.00	21.64
ATOM	1220	C	LEU	369	8.772	14.076	57.235	1.00	19.07
ATOM	1221	O	LEU	369	7.945	14.606	57.965	1.00	17.17
ATOM	1222	N	LYS	370	10.007	14.567	57.120	1.00	18.01
ATOM	1223	CA	LYS	370	10.363	15.799	57.826	1.00	19.26
ATOM	1224	CB	LYS	370	11.819	16.199	57.522	1.00	18.97
ATOM	1225	CG	LYS	370	12.888	15.349	58.203	1.00	21.31
ATOM	1226	CD	LYS	370	14.304	15.860	57.845	1.00	25.49
ATOM	1227	CE	LYS	370	14.445	17.367	58.009	1.00	25.79
ATOM	1228	NZ	LYS	370	15.878	17.841	57.879	1.00	29.87
ATOM	1229	C	LYS	370	9.440	16.949	57.388	1.00	17.68
ATOM	1230	O	LYS	370	8.950	17.717	58.203	1.00	17.05
ATOM	1231	N	ALA	371	9.209	17.075	56.081	1.00	17.98
ATOM	1232	CA	ALA	371	8.368	18.154	55.596	1.00	17.26
ATOM	1233	CB	ALA	371	8.344	18.154	54.065	1.00	19.00
ATOM	1234	C	ALA	371	6.957	17.957	56.140	1.00	15.65
ATOM	1235	O	ALA	371	6.299	18.909	56.533	1.00	17.13
ATOM	1236	N	ILE	372	6.492	16.713	56.151	1.00	14.92
ATOM	1237	CA	ILE	372	5.146	16.450	56.673	1.00	16.38
ATOM	1238	CB	ILE	372	4.743	14.956	56.430	1.00	15.28
ATOM	1239	CG2	ILE	372	3.477	14.602	57.245	1.00	17.98
ATOM	1240	CG1	ILE	372	4.566	14.730	54.915	1.00	18.14
ATOM	1241	CD1	ILE	372	4.413	13.271	54.530	1.00	18.13
ATOM	1242	C	ILE	372	5.038	16.795	58.163	1.00	16.98
ATOM	1243	O	ILE	372	4.028	17.317	58.606	1.00	16.87
ATOM	1244	N	ILE	373	6.089	16.522	58.942	1.00	14.47
ATOM	1245	CA	ILE	373	6.080	16.829	60.369	1.00	15.13
ATOM	1246	CB	ILE	373	7.392	16.251	61.042	1.00	13.81
ATOM	1247	CG2	ILE	373	7.530	16.783	62.463	1.00	15.08
ATOM	1248	CG1	ILE	373	7.340	14.717	61.052	1.00	14.66
ATOM	1249	CD1	ILE	373	8.709	14.031	61.219	1.00	17.60
ATOM	1250	C	ILE	373	5.962	18.350	60.604	1.00	15.01

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ATOM  1251  O   ILE  373      5.212  18.817  61.477  1.00 15.67
ATOM  1252  N   LEU  374      6.702  19.109  59.796  1.00 16.23
ATOM  1253  CA  LEU  374      6.688  20.557  59.880  1.00 15.91
ATOM  1254  CB  LEU  374      7.738  21.160  58.942  1.00 18.27
ATOM  1255  CG  LEU  374      7.702  22.700  58.759  1.00 19.49
ATOM  1256  CD1 LEU  374      8.184  23.403  60.044  1.00 18.70
ATOM  1257  CD2 LEU  374      8.596  23.092  57.597  1.00 19.61
ATOM  1258  C   LEU  374      5.316  21.128  59.490  1.00 17.14
ATOM  1259  O   LEU  374      4.765  21.980  60.167  1.00 16.72
ATOM  1260  N   LEU  375      4.803  20.662  58.367  1.00 17.78
ATOM  1261  CA  LEU  375      3.561  21.202  57.831  1.00 17.01
ATOM  1262  CB  LEU  375      3.573  21.071  56.301  1.00 19.06
ATOM  1263  CG  LEU  375      4.788  21.715  55.581  1.00 18.84
ATOM  1264  CD1 LEU  375      4.903  21.197  54.151  1.00 18.22
ATOM  1265  CD2 LEU  375      4.644  23.234  55.610  1.00 19.41
ATOM  1266  C   LEU  375      2.349  20.514  58.422  1.00 19.26
ATOM  1267  O   LEU  375      1.603  19.823  57.705  1.00 19.50
ATOM  1268  N   ASN  376      2.178  20.727  59.723  1.00 16.95
ATOM  1269  CA  ASN  376      1.087  20.136  60.510  1.00 19.78
ATOM  1270  CB  ASN  376      1.605  19.772  61.912  1.00 18.97
ATOM  1271  CG  ASN  376      0.537  19.124  62.780  1.00 23.13
ATOM  1272  OD1 ASN  376     -0.527  18.732  62.289  1.00 19.72
ATOM  1273  ND2 ASN  376      0.827  18.989  64.081  1.00 21.10
ATOM  1274  C   ASN  376     -0.088  21.080  60.641  1.00 17.80
ATOM  1275  O   ASN  376     -0.043  22.028  61.412  1.00 18.77
ATOM  1276  N   PRO  377     -1.188  20.820  59.909  1.00 20.03
ATOM  1277  CD  PRO  377     -1.463  19.684  59.010  1.00 19.34
ATOM  1278  CA  PRO  377     -2.342  21.728  60.011  1.00 20.40
ATOM  1279  CB  PRO  377     -3.239  21.293  58.858  1.00 18.78
ATOM  1280  CG  PRO  377     -2.979  19.796  58.774  1.00 19.22
ATOM  1281  C   PRO  377     -3.086  21.705  61.336  1.00 21.89
ATOM  1282  O   PRO  377     -3.922  22.583  61.594  1.00 22.57
ATOM  1283  N   ASP  378     -2.771  20.723  62.177  1.00 20.09
ATOM  1284  CA  ASP  378     -3.444  20.609  63.463  1.00 22.47
ATOM  1285  CB  ASP  378     -3.608  19.131  63.809  1.00 23.71
ATOM  1286  CG  ASP  378     -4.555  18.426  62.847  1.00 25.43
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ATOM 1287 OD1 ASP 378 -5.579 19.028 62.487 1.00 28.35
ATOM 1288 OD2 ASP 378 -4.289 17.283 62.443 1.00 30.58
ATOM 1289 C ASP 378 -2.823 21.403 64.603 1.00 22.30
ATOM 1290 O ASP 378 -3.265 21.309 65.760 1.00 22.98
ATOM 1291 N VAL 379 -1.793 22.181 64.279 1.00 22.51
ATOM 1292 CA VAL 379 -1.167 23.053 65.266 1.00 21.52
ATOM 1293 CB VAL 379 0.044 23.807 64.662 1.00 20.60
ATOM 1294 CG1 VAL 379 0.424 25.004 65.532 1.00 22.27
ATOM 1295 CG2 VAL 379 1.226 22.848 64.516 1.00 22.31
ATOM 1296 C VAL 379 -2.255 24.048 65.658 1.00 23.83
ATOM 1297 O VAL 379 -2.918 24.655 64.793 1.00 25.06
ATOM 1298 N LYS 380 -2.460 24.212 66.958 1.00 23.33
ATOM 1299 CA LYS 380 -3.490 25.124 67.430 1.00 24.49
ATOM 1300 CB LYS 380 -3.797 24.829 68.904 1.00 25.21
ATOM 1301 CG LYS 380 -4.182 23.365 69.131 1.00 28.03
ATOM 1302 CD LYS 380 -4.460 23.035 70.594 1.00 30.82
ATOM 1303 CE LYS 380 -4.728 21.536 70.758 1.00 31.68
ATOM 1304 NZ LYS 380 -4.904 21.079 72.177 1.00 33.50
ATOM 1305 C LYS 380 -3.055 26.573 67.250 1.00 24.85
ATOM 1306 O LYS 380 -1.874 26.891 67.408 1.00 25.55
ATOM 1307 N GLY 381 -3.988 27.445 66.861 1.00 24.69
ATOM 1308 CA GLY 381 -3.647 28.852 66.704 1.00 26.29
ATOM 1309 C GLY 381 -3.384 29.378 65.295 1.00 25.30
ATOM 1310 O GLY 381 -3.246 30.598 65.093 1.00 27.29
ATOM 1311 N LEU 382 -3.313 28.490 64.311 1.00 26.35
ATOM 1312 CA LEU 382 -3.054 28.914 62.941 1.00 26.95
ATOM 1313 CB LEU 382 -2.997 27.706 61.995 1.00 25.01
ATOM 1314 CG LEU 382 -1.865 26.700 62.265 1.00 24.87
ATOM 1315 CD1 LEU 382 -2.011 25.507 61.314 1.00 24.53
ATOM 1316 CD2 LEU 382 -0.518 27.384 62.064 1.00 24.40
ATOM 1317 C LEU 382 -4.120 29.885 62.428 1.00 28.77
ATOM 1318 O LEU 382 -5.310 29.719 62.695 1.00 28.39
ATOM 1319 N LYS 383 -3.660 30.881 61.681 1.00 30.83
ATOM 1320 CA LYS 383 -4.518 31.894 61.078 1.00 32.60
ATOM 1321 CB LYS 383 -3.670 33.104 60.699 1.00 35.65
ATOM 1322 CG LYS 383 -4.352 34.121 59.788 1.00 40.31

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ATOM  1323  CD  LYS  383     -5.044  35.203  60.589  1.00 42.92
ATOM  1324  CE  LYS  383     -5.436  36.376  59.702  1.00 43.80
ATOM  1325  NZ  LYS  383     -6.040  37.476  60.505  1.00 44.52
ATOM  1326  C   LYS  383     -5.159  31.313  59.819  1.00 32.46
ATOM  1327  O   LYS  383     -6.374  31.411  59.620  1.00 33.42
ATOM  1328  N   ASN  384     -4.332  30.700  58.977  1.00 30.19
ATOM  1329  CA  ASN  384     -4.794  30.118  57.720  1.00 29.86
ATOM  1330  CB  ASN  384     -4.154  30.854  56.549  1.00 32.74
ATOM  1331  CG  ASN  384     -4.460  32.336  56.570  1.00 36.46
ATOM  1332  OD1 ASN  384     -5.625  32.730  56.585  1.00 39.59
ATOM  1333  ND2 ASN  384     -3.418  33.166  56.583  1.00 37.88
ATOM  1334  C   ASN  384     -4.466  28.636  57.636  1.00 26.29
ATOM  1335  O   ASN  384     -3.558  28.229  56.912  1.00 26.38
ATOM  1336  N   ARG  385     -5.218  27.845  58.387  1.00 24.62
ATOM  1337  CA  ARG  385     -5.005  26.406  58.431  1.00 24.85
ATOM  1338  CB  ARG  385     -5.994  25.779  59.413  1.00 24.62
ATOM  1339  CG  ARG  385     -5.910  24.275  59.561  1.00 27.77
ATOM  1340  CD  ARG  385     -6.705  23.839  60.785  1.00 30.37
ATOM  1341  NE  ARG  385     -5.976  24.188  62.004  1.00 31.78
ATOM  1342  CZ  ARG  385     -6.329  25.148  62.849  1.00 31.80
ATOM  1343  NH1 ARG  385     -7.432  25.867  62.629  1.00 31.71
ATOM  1344  NH2 ARG  385     -5.542  25.426  63.886  1.00 28.60
ATOM  1345  C   ARG  385     -5.079  25.727  57.070  1.00 24.38
ATOM  1346  O   ARG  385     -4.289  24.824  56.783  1.00 24.23
ATOM  1347  N   GLN  386     -6.003  26.165  56.214  1.00 24.39
ATOM  1348  CA  GLN  386     -6.128  25.542  54.906  1.00 25.99
ATOM  1349  CB  GLN  386     -7.320  26.124  54.128  1.00 29.68
ATOM  1350  CG  GLN  386     -7.256  27.619  53.863  1.00 34.93
ATOM  1351  CD  GLN  386     -7.246  28.442  55.136  1.00 37.35
ATOM  1352  OE1 GLN  386     -8.016  28.183  56.072  1.00 39.44
ATOM  1353  NE2 GLN  386     -6.373  29.443  55.183  1.00 39.95
ATOM  1354  C   GLN  386     -4.867  25.646  54.067  1.00 24.30
ATOM  1355  O   GLN  386     -4.561  24.727  53.318  1.00 25.10
ATOM  1356  N   GLU  387     -4.140  26.752  54.182  1.00 25.50
ATOM  1357  CA  GLU  387     -2.907  26.905  53.413  1.00 25.38
ATOM  1358  CB  GLU  387     -2.358  28.328  53.594  1.00 29.21
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ATOM 1359 CG GLU 387 -3.234 29.420 52.915 1.00 33.12
ATOM 1360 CD GLU 387 -2.845 30.838 53.284 1.00 37.28
ATOM 1361 OE1 GLU 387 -1.634 31.125 53.407 1.00 40.75
ATOM 1362 OE2 GLU 387 -3.750 31.691 53.436 1.00 38.95
ATOM 1363 C GLU 387 -1.877 25.841 53.852 1.00 25.54
ATOM 1364 O GLU 387 -1.097 25.329 53.030 1.00 24.67
ATOM 1365 N VAL 388 -1.897 25.476 55.132 1.00 24.28
ATOM 1366 CA VAL 388 -0.960 24.447 55.617 1.00 21.40
ATOM 1367 CB VAL 388 -0.845 24.439 57.168 1.00 19.68
ATOM 1368 CG1 VAL 388 0.182 23.410 57.597 1.00 22.22
ATOM 1369 CG2 VAL 388 -0.477 25.824 57.691 1.00 20.28
ATOM 1370 C VAL 388 -1.444 23.076 55.178 1.00 22.10
ATOM 1371 O VAL 388 -0.666 22.211 54.782 1.00 21.10
ATOM 1372 N GLU 389 -2.750 22.859 55.243 1.00 22.00
ATOM 1373 CA GLU 389 -3.284 21.577 54.825 1.00 21.41
ATOM 1374 CB GLU 389 -4.801 21.538 54.987 1.00 22.76
ATOM 1375 CG GLU 389 -5.358 20.146 54.988 1.00 31.47
ATOM 1376 CD GLU 389 -6.793 20.093 55.471 1.00 36.14
ATOM 1377 OE1 GLU 389 -7.160 20.927 56.334 1.00 39.74
ATOM 1378 OE2 GLU 389 -7.540 19.204 55.006 1.00 39.63
ATOM 1379 C GLU 389 -2.936 21.294 53.382 1.00 19.32
ATOM 1380 O GLU 389 -2.653 20.155 53.025 1.00 21.32
ATOM 1381 N VAL 390 -3.001 22.313 52.534 1.00 19.72
ATOM 1382 CA VAL 390 -2.685 22.148 51.125 1.00 19.82
ATOM 1383 CB VAL 390 -2.950 23.447 50.316 1.00 19.77
ATOM 1384 CG1 VAL 390 -2.307 23.344 48.919 1.00 22.22
ATOM 1385 CG2 VAL 390 -4.442 23.652 50.169 1.00 23.95
ATOM 1386 C VAL 390 -1.231 21.744 50.924 1.00 20.27
ATOM 1387 O VAL 390 -0.924 20.894 50.093 1.00 20.79
ATOM 1388 N LEU 391 -0.334 22.345 51.699 1.00 21.06
ATOM 1389 CA LEU 391 1.078 22.004 51.552 1.00 19.84
ATOM 1390 CB LEU 391 1.951 22.982 52.328 1.00 20.90
ATOM 1391 CG LEU 391 1.895 24.438 51.836 1.00 21.65
ATOM 1392 CD1 LEU 391 2.846 25.283 52.673 1.00 23.70
ATOM 1393 CD2 LEU 391 2.260 24.515 50.351 1.00 25.56
ATOM 1394 C LEU 391 1.327 20.583 52.031 1.00 19.59

ATOM	1395	O	LEU	391	2.090	19.837	51.421	1.00	19.63	
ATOM	1396	N	ARG	392	0.680	20.192	53.130	0.50	19.30	AC1
ATOM	1397	CA	ARG	392	0.862	18.823	53.628	0.50	19.65	AC1
ATOM	1398	CB	ARG	392	0.212	18.620	55.016	0.50	19.22	AC1
ATOM	1399	CG	ARG	392	0.060	17.123	55.382	0.50	18.74	AC1
ATOM	1400	CD	ARG	392	-0.380	16.857	56.840	0.50	19.04	AC1
ATOM	1401	NE	ARG	392	0.710	17.001	57.811	0.50	18.30	AC1
ATOM	1402	CZ	ARG	392	0.739	16.427	59.020	0.50	18.32	AC1
ATOM	1403	NH1	ARG	392	-0.262	15.660	59.432	0.50	18.09	AC1
ATOM	1404	NH2	ARG	392	1.783	16.606	59.826	0.50	13.08	AC1
ATOM	1405	C	ARG	392	0.259	17.833	52.624	0.50	19.79	AC1
ATOM	1406	O	ARG	392	0.768	16.730	52.453	0.50	19.90	AC1
ATOM	1407	N	GLU	393	-0.839	18.220	51.976	1.00	19.51	
ATOM	1408	CA	GLU	393	-1.484	17.355	50.979	1.00	21.32	
ATOM	1409	CB	GLU	393	-2.858	17.922	50.575	1.00	23.83	
ATOM	1410	CG	GLU	393	-3.631	17.066	49.588	1.00	29.44	
ATOM	1411	CD	GLU	393	-4.209	15.767	50.173	1.00	34.23	
ATOM	1412	OE1	GLU	393	-3.940	15.434	51.348	1.00	34.71	
ATOM	1413	OE2	GLU	393	-4.952	15.071	49.433	1.00	37.12	
ATOM	1414	C	GLU	393	-0.556	17.210	49.763	1.00	21.12	
ATOM	1415	O	GLU	393	-0.486	16.147	49.157	1.00	20.35	
ATOM	1416	N	LYS	394	0.143	18.287	49.395	1.00	19.98	
ATOM	1417	CA	LYS	394	1.102	18.186	48.302	1.00	21.24	
ATOM	1418	CB	LYS	394	1.787	19.519	48.048	1.00	22.05	
ATOM	1419	CG	LYS	394	0.903	20.468	47.258	1.00	24.02	
ATOM	1420	CD	LYS	394	1.608	21.778	46.964	1.00	25.62	
ATOM	1421	CE	LYS	394	0.690	22.711	46.199	1.00	28.47	
ATOM	1422	NZ	LYS	394	1.369	24.012	45.959	1.00	30.41	
ATOM	1423	C	LYS	394	2.153	17.137	48.667	1.00	22.08	
ATOM	1424	O	LYS	394	2.555	16.341	47.825	1.00	20.82	
ATOM	1425	N	MET	395	2.590	17.136	49.932	1.00	21.43	
ATOM	1426	CA	MET	395	3.607	16.166	50.369	1.00	21.13	
ATOM	1427	CB	MET	395	4.177	16.520	51.746	1.00	24.05	
ATOM	1428	CG	MET	395	5.100	17.680	51.738	1.00	24.66	
ATOM	1429	SD	MET	395	6.457	17.503	50.571	1.00	27.36	
ATOM	1430	CE	MET	395	6.985	15.797	50.738	1.00	23.91	

ATOM	1431	C	MET	395	3.121	14.744	50.417	1.00	20.46
ATOM	1432	O	MET	395	3.872	13.832	50.095	1.00	22.42
ATOM	1433	N	PHE	396	1.862	14.542	50.827	1.00	20.87
ATOM	1434	CA	PHE	396	1.285	13.202	50.858	1.00	21.65
ATOM	1435	CB	PHE	396	-0.176	13.203	51.374	1.00	20.90
ATOM	1436	CG	PHE	396	-0.320	13.286	52.875	1.00	22.60
ATOM	1437	CD1	PHE	396	0.733	12.996	53.727	1.00	22.79
ATOM	1438	CD2	PHE	396	-1.544	13.640	53.436	1.00	23.58
ATOM	1439	CE1	PHE	396	0.570	13.063	55.116	1.00	20.29
ATOM	1440	CE2	PHE	396	-1.712	13.702	54.826	1.00	23.72
ATOM	1441	CZ	PHE	396	-0.655	13.416	55.669	1.00	22.24
ATOM	1442	C	PHE	396	1.281	12.652	49.429	1.00	22.43
ATOM	1443	O	PHE	396	1.635	11.494	49.215	1.00	21.80
ATOM	1444	N	LEU	397	0.844	13.462	48.458	1.00	22.96
ATOM	1445	CA	LEU	397	0.813	13.022	47.061	1.00	21.97
ATOM	1446	CB	LEU	397	0.139	14.099	46.176	1.00	22.88
ATOM	1447	CG	LEU	397	-1.385	14.161	46.354	1.00	23.93
ATOM	1448	CD1	LEU	397	-1.981	15.078	45.315	1.00	25.27
ATOM	1449	CD2	LEU	397	-1.972	12.759	46.190	1.00	25.99
ATOM	1450	C	LEU	397	2.233	12.705	46.560	1.00	24.94
ATOM	1451	O	LEU	397	2.450	11.692	45.873	1.00	25.61
ATOM	1452	N	CYS	398	3.195	13.548	46.924	1.00	23.80
ATOM	1453	CA	CYS	398	4.593	13.333	46.519	1.00	26.51
ATOM	1454	CB	CYS	398	5.509	14.454	47.041	1.00	28.87
ATOM	1455	SG	CYS	398	5.551	15.910	46.032	1.00	39.48
ATOM	1456	C	CYS	398	5.111	12.027	47.090	1.00	25.35
ATOM	1457	O	CYS	398	5.738	11.221	46.399	1.00	25.03
ATOM	1458	N	LEU	399	4.861	11.821	48.371	1.00	24.81
ATOM	1459	CA	LEU	399	5.366	10.620	49.009	1.00	24.04
ATOM	1460	CB	LEU	399	5.232	10.739	50.530	1.00	24.26
ATOM	1461	CG	LEU	399	5.806	9.580	51.344	1.00	24.01
ATOM	1462	CD1	LEU	399	7.281	9.343	50.985	1.00	22.08
ATOM	1463	CD2	LEU	399	5.672	9.931	52.821	1.00	22.85
ATOM	1464	C	LEU	399	4.715	9.352	48.518	1.00	26.35
ATOM	1465	O	LEU	399	5.398	8.363	48.267	1.00	25.02
ATOM	1466	N	ASP	400	3.391	9.377	48.361	1.00	27.30

ATOM	1467	CA	ASP	400	2.680	8.200	47.874	1.00	29.09
ATOM	1468	CB	ASP	400	1.179	8.490	47.772	1.00	31.25
ATOM	1469	CG	ASP	400	0.379	7.258	47.400	1.00	34.75
ATOM	1470	OD1	ASP	400	0.236	6.356	48.252	1.00	35.16
ATOM	1471	OD2	ASP	400	-0.091	7.188	46.250	1.00	38.49
ATOM	1472	C	ASP	400	3.217	7.816	46.497	1.00	28.91
ATOM	1473	O	ASP	400	3.436	6.642	46.212	1.00	29.66
ATOM	1474	N	GLU	401	3.420	8.813	45.644	1.00	28.16
ATOM	1475	CA	GLU	401	3.936	8.577	44.299	1.00	29.87
ATOM	1476	CB	GLU	401	4.052	9.895	43.533	1.00	32.50
ATOM	1477	CG	GLU	401	4.735	9.751	42.180	1.00	38.83
ATOM	1478	CD	GLU	401	4.784	11.048	41.406	1.00	42.93
ATOM	1479	OE1	GLU	401	5.449	12.003	41.865	1.00	45.46
ATOM	1480	OE2	GLU	401	4.147	11.114	40.334	1.00	45.87
ATOM	1481	C	GLU	401	5.308	7.911	44.360	1.00	31.19
ATOM	1482	O	GLU	401	5.574	6.926	43.650	1.00	31.37
ATOM	1483	N	TYR	402	6.171	8.444	45.224	1.00	28.55
ATOM	1484	CA	TYR	402	7.516	7.918	45.365	1.00	29.01
ATOM	1485	CB	TYR	402	8.314	8.737	46.384	1.00	27.40
ATOM	1486	CG	TYR	402	9.667	8.134	46.659	1.00	27.45
ATOM	1487	CD1	TYR	402	9.849	7.238	47.709	1.00	27.18
ATOM	1488	CE1	TYR	402	11.087	6.635	47.933	1.00	28.15
ATOM	1489	CD2	TYR	402	10.747	8.419	45.834	1.00	27.22
ATOM	1490	CE2	TYR	402	11.996	7.820	46.050	1.00	30.03
ATOM	1491	CZ	TYR	402	12.147	6.936	47.097	1.00	30.78
ATOM	1492	OH	TYR	402	13.374	6.358	47.316	1.00	31.66
ATOM	1493	C	TYR	402	7.503	6.453	45.769	1.00	30.16
ATOM	1494	O	TYR	402	8.206	5.641	45.187	1.00	29.67
ATOM	1495	N	CYS	403	6.700	6.113	46.763	1.00	30.42
ATOM	1496	CA	CYS	403	6.616	4.739	47.215	1.00	34.32
ATOM	1497	CB	CYS	403	5.691	4.650	48.430	1.00	33.37
ATOM	1498	SG	CYS	403	6.357	5.485	49.920	1.00	31.63
ATOM	1499	C	CYS	403	6.116	3.820	46.104	1.00	36.81
ATOM	1500	O	CYS	403	6.612	2.703	45.936	1.00	36.95
ATOM	1501	N	ARG	404	5.140	4.289	45.335	1.00	39.50
ATOM	1502	CA	ARG	404	4.597	3.453	44.271	1.00	42.67

ATOM	1503	CB	ARG	404	3.280	4.045	43.746	1.00	43.44
ATOM	1504	CG	ARG	404	2.135	3.802	44.718	1.00	46.08
ATOM	1505	CD	ARG	404	0.746	4.164	44.188	1.00	46.89
ATOM	1506	NE	ARG	404	0.490	5.602	44.159	1.00	46.69
ATOM	1507	CZ	ARG	404	0.733	6.386	43.116	1.00	47.48
ATOM	1508	NH1	ARG	404	1.241	5.874	42.002	1.00	48.94
ATOM	1509	NH2	ARG	404	0.462	7.684	43.181	1.00	48.22
ATOM	1510	C	ARG	404	5.578	3.206	43.137	1.00	43.67
ATOM	1511	O	ARG	404	5.640	2.102	42.598	1.00	44.97
ATOM	1512	N	ARG	405	6.356	4.220	42.785	1.00	45.45
ATOM	1513	CA	ARG	405	7.330	4.098	41.710	1.00	47.72
ATOM	1514	CB	ARG	405	7.700	5.481	41.167	1.00	49.80
ATOM	1515	CG	ARG	405	6.535	6.298	40.624	1.00	53.09
ATOM	1516	CD	ARG	405	7.005	7.695	40.233	1.00	56.62
ATOM	1517	NE	ARG	405	5.931	8.506	39.661	1.00	59.35
ATOM	1518	CZ	ARG	405	5.356	8.263	38.488	1.00	60.20
ATOM	1519	NH1	ARG	405	5.753	7.231	37.756	1.00	61.80
ATOM	1520	NH2	ARG	405	4.382	9.049	38.046	1.00	60.75
ATOM	1521	C	ARG	405	8.609	3.410	42.166	1.00	48.23
ATOM	1522	O	ARG	405	9.078	2.464	41.528	1.00	48.90
ATOM	1523	N	SER	406	9.163	3.891	43.278	1.00	47.66
ATOM	1524	CA	SER	406	10.421	3.382	43.819	1.00	48.66
ATOM	1525	CB	SER	406	11.099	4.477	44.638	1.00	49.49
ATOM	1526	OG	SER	406	11.118	5.698	43.919	1.00	51.64
ATOM	1527	C	SER	406	10.336	2.112	44.656	1.00	48.77
ATOM	1528	O	SER	406	11.355	1.507	44.968	1.00	48.91
ATOM	1529	N	ARG	407	9.129	1.711	45.026	1.00	49.27
ATOM	1530	CA	ARG	407	8.948	0.500	45.813	1.00	50.47
ATOM	1531	CB	ARG	407	9.106	0.811	47.302	1.00	52.25
ATOM	1532	CG	ARG	407	10.476	0.434	47.849	1.00	54.88
ATOM	1533	CD	ARG	407	10.942	1.401	48.918	1.00	55.39
ATOM	1534	NE	ARG	407	12.157	0.927	49.573	1.00	56.11
ATOM	1535	CZ	ARG	407	12.885	1.653	50.416	1.00	56.40
ATOM	1536	NH1	ARG	407	12.524	2.895	50.707	1.00	56.21
ATOM	1537	NH2	ARG	407	13.973	1.133	50.972	1.00	55.90
ATOM	1538	C	ARG	407	7.586	-0.110	45.535	1.00	50.00

ATOM 1539 O ARG 407 6.847 -0.468 46.451 1.00 50.06
ATOM 1540 N SER 408 7.279 -0.233 44.248 1.00 49.76
ATOM 1541 CA SER 408 6.010 -0.777 43.782 1.00 49.98
ATOM 1542 CB SER 408 6.060 -0.957 42.262 1.00 50.23
ATOM 1543 OG SER 408 7.129 -1.806 41.880 1.00 50.48
ATOM 1544 C SER 408 5.622 -2.100 44.439 1.00 49.86
ATOM 1545 O SER 408 4.444 -2.354 44.698 1.00 50.10
ATOM 1546 N SER 409 6.620 -2.933 44.706 1.00 50.01
ATOM 1547 CA SER 409 6.412 -4.245 45.307 1.00 49.71
ATOM 1548 CB SER 409 7.704 -5.055 45.217 1.00 50.85
ATOM 1549 OG SER 409 8.799 -4.306 45.730 1.00 52.55
ATOM 1550 C SER 409 5.954 -4.195 46.758 1.00 49.15
ATOM 1551 O SER 409 5.476 -5.195 47.300 1.00 48.48
ATOM 1552 N GLU 410 6.095 -3.035 47.392 1.00 47.66
ATOM 1553 CA GLU 410 5.701 -2.912 48.785 1.00 45.50
ATOM 1554 CB GLU 410 6.787 -2.197 49.577 1.00 46.29
ATOM 1555 CG GLU 410 8.079 -2.980 49.712 1.00 47.76
ATOM 1556 CD GLU 410 9.074 -2.261 50.592 1.00 48.13
ATOM 1557 OE1 GLU 410 10.155 -1.882 50.092 1.00 49.66
ATOM 1558 OE2 GLU 410 8.761 -2.063 51.784 1.00 48.57
ATOM 1559 C GLU 410 4.373 -2.197 48.973 1.00 44.10
ATOM 1560 O GLU 410 4.311 -0.974 49.114 1.00 41.70
ATOM 1561 N GLU 411 3.306 -2.985 48.986 1.00 42.76
ATOM 1562 CA GLU 411 1.973 -2.451 49.154 1.00 41.57
ATOM 1563 CB GLU 411 0.945 -3.529 48.814 1.00 44.42
ATOM 1564 CG GLU 411 1.166 -4.132 47.439 1.00 48.49
ATOM 1565 CD GLU 411 0.151 -5.191 47.100 1.00 49.60
ATOM 1566 OE1 GLU 411 0.111 -6.226 47.806 1.00 49.80
ATOM 1567 OE2 GLU 411 -0.605 -4.979 46.129 1.00 50.58
ATOM 1568 C GLU 411 1.805 -2.000 50.594 1.00 38.78
ATOM 1569 O GLU 411 2.254 -2.682 51.526 1.00 38.53
ATOM 1570 N GLY 412 1.170 -0.845 50.768 1.00 34.78
ATOM 1571 CA GLY 412 0.953 -0.313 52.103 1.00 32.19
ATOM 1572 C GLY 412 2.163 0.402 52.695 1.00 29.28
ATOM 1573 O GLY 412 2.133 0.770 53.865 1.00 28.68
ATOM 1574 N ARG 413 3.207 0.625 51.901 1.00 28.70

ATOM	1575	CA	ARG	413	4.413	1.286	52.407	1.00	27.65
ATOM	1576	CB	ARG	413	5.513	1.319	51.348	1.00	29.50
ATOM	1577	CG	ARG	413	6.850	1.839	51.905	1.00	29.56
ATOM	1578	CD	ARG	413	8.004	1.721	50.903	1.00	32.68
ATOM	1579	NE	ARG	413	9.242	2.244	51.484	1.00	34.48
ATOM	1580	CZ	ARG	413	9.951	1.632	52.433	1.00	35.49
ATOM	1581	NH1	ARG	413	9.569	0.454	52.914	1.00	34.87
ATOM	1582	NH2	ARG	413	11.036	2.221	52.929	1.00	35.73
ATOM	1583	C	ARG	413	4.153	2.715	52.874	1.00	27.61
ATOM	1584	O	ARG	413	4.656	3.142	53.911	1.00	26.64
ATOM	1585	N	PHE	414	3.377	3.447	52.091	1.00	27.23
ATOM	1586	CA	PHE	414	3.025	4.829	52.406	1.00	25.72
ATOM	1587	CB	PHE	414	2.109	5.368	51.290	1.00	27.69
ATOM	1588	CG	PHE	414	1.553	6.756	51.552	1.00	26.95
ATOM	1589	CD1	PHE	414	2.359	7.882	51.454	1.00	28.43
ATOM	1590	CD2	PHE	414	0.217	6.921	51.891	1.00	29.19
ATOM	1591	CE1	PHE	414	1.842	9.165	51.692	1.00	28.49
ATOM	1592	CE2	PHE	414	-0.315	8.199	52.134	1.00	29.46
ATOM	1593	CZ	PHE	414	0.503	9.325	52.033	1.00	28.75
ATOM	1594	C	PHE	414	2.336	4.891	53.777	1.00	26.40
ATOM	1595	O	PHE	414	2.691	5.702	54.637	1.00	26.65
ATOM	1596	N	ALA	415	1.355	4.027	53.997	1.00	25.07
ATOM	1597	CA	ALA	415	0.652	4.002	55.271	1.00	24.63
ATOM	1598	CB	ALA	415	-0.531	3.028	55.193	1.00	23.72
ATOM	1599	C	ALA	415	1.572	3.622	56.436	1.00	24.02
ATOM	1600	O	ALA	415	1.433	4.142	57.547	1.00	23.15
ATOM	1601	N	ALA	416	2.518	2.722	56.174	1.00	24.35
ATOM	1602	CA	ALA	416	3.448	2.270	57.205	1.00	24.54
ATOM	1603	CB	ALA	416	4.313	1.143	56.666	1.00	24.42
ATOM	1604	C	ALA	416	4.319	3.436	57.639	1.00	23.97
ATOM	1605	O	ALA	416	4.544	3.646	58.832	1.00	25.89
ATOM	1606	N	LEU	417	4.799	4.192	56.664	1.00	23.99
ATOM	1607	CA	LEU	417	5.638	5.348	56.952	1.00	23.65
ATOM	1608	CB	LEU	417	6.056	6.013	55.651	1.00	23.88
ATOM	1609	CG	LEU	417	6.940	5.132	54.768	1.00	22.81
ATOM	1610	CD1	LEU	417	7.104	5.745	53.381	1.00	25.97

ATOM	1611	CD2	LEU	417	8.313	4.978	55.464	1.00	24.86
ATOM	1612	C	LEU	417	4.894	6.346	57.843	1.00	23.64
ATOM	1613	O	LEU	417	5.434	6.825	58.851	1.00	24.26
ATOM	1614	N	LEU	418	3.635	6.632	57.517	1.00	22.96
ATOM	1615	CA	LEU	418	2.896	7.617	58.305	1.00	22.78
ATOM	1616	CB	LEU	418	1.555	7.961	57.622	1.00	22.19
ATOM	1617	CG	LEU	418	1.632	8.536	56.193	1.00	22.93
ATOM	1618	CD1	LEU	418	0.232	8.983	55.715	1.00	23.88
ATOM	1619	CD2	LEU	418	2.554	9.749	56.179	1.00	23.65
ATOM	1620	C	LEU	418	2.646	7.201	59.762	1.00	24.12
ATOM	1621	O	LEU	418	2.372	8.046	60.620	1.00	22.61
ATOM	1622	N	LEU	419	2.706	5.901	60.049	1.00	25.06
ATOM	1623	CA	LEU	419	2.496	5.440	61.404	1.00	27.92
ATOM	1624	CB	LEU	419	2.406	3.909	61.451	1.00	31.65
ATOM	1625	CG	LEU	419	1.114	3.343	60.884	1.00	34.11
ATOM	1626	CD1	LEU	419	1.026	1.848	61.218	1.00	36.06
ATOM	1627	CD2	LEU	419	-0.068	4.081	61.480	1.00	34.83
ATOM	1628	C	LEU	419	3.594	5.891	62.360	1.00	29.85
ATOM	1629	O	LEU	419	3.400	5.885	63.574	1.00	31.55
ATOM	1630	N	ARG	420	4.736	6.296	61.828	1.00	31.33
ATOM	1631	CA	ARG	420	5.801	6.725	62.718	1.00	31.87
ATOM	1632	CB	ARG	420	7.145	6.755	61.985	1.00	32.74
ATOM	1633	CG	ARG	420	7.648	5.387	61.490	1.00	33.67
ATOM	1634	CD	ARG	420	7.856	4.364	62.622	1.00	36.93
ATOM	1635	NE	ARG	420	6.709	3.481	62.820	1.00	35.35
ATOM	1636	CZ	ARG	420	6.179	3.194	64.003	1.00	37.82
ATOM	1637	NH1	ARG	420	6.692	3.714	65.116	1.00	39.26
ATOM	1638	NH2	ARG	420	5.112	2.408	64.079	1.00	39.04
ATOM	1639	C	ARG	420	5.477	8.092	63.303	1.00	32.15
ATOM	1640	O	ARG	420	5.995	8.456	64.362	1.00	31.60
ATOM	1641	N	LEU	421	4.591	8.845	62.655	1.00	30.38
ATOM	1642	CA	LEU	421	4.278	10.175	63.164	1.00	29.53
ATOM	1643	CB	LEU	421	3.519	10.976	62.121	1.00	30.72
ATOM	1644	CG	LEU	421	4.322	11.027	60.808	1.00	31.31
ATOM	1645	CD1	LEU	421	3.645	12.019	59.885	1.00	32.38
ATOM	1646	CD2	LEU	421	5.800	11.411	61.053	1.00	31.74

ATOM	1647	C	LEU	421	3.582	10.256	64.521	1.00	28.39
ATOM	1648	O	LEU	421	3.977	11.061	65.363	1.00	26.36
ATOM	1649	N	PRO	422	2.533	9.446	64.762	1.00	27.69
ATOM	1650	CD	PRO	422	1.678	8.672	63.839	1.00	27.47
ATOM	1651	CA	PRO	422	1.915	9.559	66.090	1.00	26.04
ATOM	1652	CB	PRO	422	0.717	8.603	66.005	1.00	28.29
ATOM	1653	CG	PRO	422	0.350	8.664	64.557	1.00	28.91
ATOM	1654	C	PRO	422	2.906	9.143	67.198	1.00	25.36
ATOM	1655	O	PRO	422	2.832	9.637	68.322	1.00	24.06
ATOM	1656	N	ALA	423	3.821	8.228	66.872	1.00	24.34
ATOM	1657	CA	ALA	423	4.817	7.779	67.840	1.00	22.88
ATOM	1658	CB	ALA	423	5.589	6.599	67.273	1.00	26.29
ATOM	1659	C	ALA	423	5.765	8.942	68.158	1.00	24.20
ATOM	1660	O	ALA	423	6.094	9.197	69.315	1.00	22.14
ATOM	1661	N	LEU	424	6.212	9.640	67.119	1.00	22.92
ATOM	1662	CA	LEU	424	7.103	10.773	67.309	1.00	22.78
ATOM	1663	CB	LEU	424	7.512	11.306	65.936	1.00	23.40
ATOM	1664	CG	LEU	424	8.405	12.531	65.875	1.00	24.54
ATOM	1665	CD1	LEU	424	9.777	12.226	66.517	1.00	22.52
ATOM	1666	CD2	LEU	424	8.589	12.892	64.405	1.00	22.78
ATOM	1667	C	LEU	424	6.422	11.861	68.153	1.00	22.46
ATOM	1668	O	LEU	424	7.036	12.468	69.038	1.00	21.68
ATOM	1669	N	ARG	425	5.136	12.101	67.900	1.00	22.38
ATOM	1670	CA	ARG	425	4.386	13.095	68.663	1.00	23.67
ATOM	1671	CB	ARG	425	2.969	13.240	68.087	1.00	26.56
ATOM	1672	CG	ARG	425	2.066	14.140	68.903	1.00	30.90
ATOM	1673	CD	ARG	425	0.977	14.732	68.031	1.00	36.25
ATOM	1674	NE	ARG	425	0.469	13.774	67.044	1.00	40.86
ATOM	1675	CZ	ARG	425	-0.070	12.592	67.339	1.00	42.76
ATOM	1676	NH1	ARG	425	-0.183	12.196	68.604	1.00	46.63
ATOM	1677	NH2	ARG	425	-0.498	11.800	66.367	1.00	44.97
ATOM	1678	C	ARG	425	4.309	12.737	70.150	1.00	21.12
ATOM	1679	O	ARG	425	4.418	13.604	71.021	1.00	21.30
ATOM	1680	N	SER	426	4.124	11.452	70.436	1.00	19.60
ATOM	1681	CA	SER	426	4.021	10.989	71.820	1.00	19.49
ATOM	1682	CB	SER	426	3.534	9.539	71.855	1.00	20.63

ATOM	1683	OG	SER	426	3.491	9.086	73.198	1.00	23.17	
ATOM	1684	C	SER	426	5.374	11.096	72.535	1.00	17.38	
ATOM	1685	O	SER	426	5.458	11.496	73.698	1.00	18.97	
ATOM	1686	N	ILE	427	6.419	10.742	71.812	1.00	18.11	
ATOM	1687	CA	ILE	427	7.770	10.812	72.368	1.00	15.88	
ATOM	1688	CB	ILE	427	8.763	10.095	71.449	1.00	15.75	
ATOM	1689	CG2	ILE	427	10.213	10.351	71.913	1.00	17.78	
ATOM	1690	CG1	ILE	427	8.479	8.591	71.526	1.00	18.23	
ATOM	1691	CD1	ILE	427	9.082	7.789	70.440	1.00	20.33	
ATOM	1692	C	ILE	427	8.146	12.272	72.599	1.00	16.69	
ATOM	1693	O	ILE	427	8.779	12.589	73.606	1.00	16.41	
ATOM	1694	N	SER	428	7.767	13.159	71.685	1.00	17.02	
ATOM	1695	CA	SER	428	8.059	14.590	71.884	1.00	17.37	
ATOM	1696	CB	SER	428	7.636	15.393	70.633	1.00	18.11	
ATOM	1697	OG	SER	428	7.745	16.794	70.876	1.00	19.14	
ATOM	1698	C	SER	428	7.377	15.138	73.154	1.00	18.08	
ATOM	1699	O	SER	428	7.968	15.916	73.928	1.00	16.98	
ATOM	1700	N	LEU	429	6.134	14.741	73.425	1.00	18.84	
ATOM	1701	CA	LEU	429	5.518	15.249	74.633	1.00	19.23	
ATOM	1702	CB	LEU	429	4.054	14.807	74.723	1.00	22.17	
ATOM	1703	CG	LEU	429	3.187	15.432	73.625	1.00	25.96	
ATOM	1704	CD1	LEU	429	1.800	14.809	73.624	1.00	28.92	
ATOM	1705	CD2	LEU	429	3.087	16.943	73.855	1.00	29.57	
ATOM	1706	C	LEU	429	6.296	14.782	75.860	1.00	17.99	
ATOM	1707	O	LEU	429	6.465	15.527	76.816	1.00	18.52	
ATOM	1708	N	LYS	430	6.778	13.544	75.830	1.00	18.39	
ATOM	1709	CA	LYS	430	7.540	13.047	76.957	1.00	17.66	
ATOM	1710	CB	LYS	430	7.780	11.544	76.826	1.00	19.73	
ATOM	1711	CG	LYS	430	8.539	10.975	78.020	1.00	23.74	
ATOM	1712	CD	LYS	430	7.625	11.004	79.260	1.00	27.95	
ATOM	1713	CE	LYS	430	8.192	10.194	80.414	1.00	34.36	
ATOM	1714	NZ	LYS	430	7.167	10.122	81.490	1.00	36.64	
ATOM	1715	C	LYS	430	8.865	13.795	77.077	1.00	18.37	
ATOM	1716	O	LYS	430	9.346	14.034	78.191	1.00	18.47	
ATOM	1717	N	SER	431	9.435	14.174	75.936	0.50	17.09	AC1
ATOM	1718	CA	SER	431	10.693	14.931	75.919	0.50	18.08	AC1

ATOM	1719	CB	SER	431	11.102	15.238	74.471	0.50	17.50	AC1
ATOM	1720	OG	SER	431	12.180	16.159	74.413	0.50	19.63	AC1
ATOM	1721	C	SER	431	10.472	16.244	76.663	0.50	18.02	AC1
ATOM	1722	O	SER	431	11.297	16.668	77.464	0.50	17.75	AC1
ATOM	1723	N	PHE	432	9.326	16.875	76.415	1.00	17.68	
ATOM	1724	CA	PHE	432	9.020	18.162	77.057	1.00	17.81	
ATOM	1725	CB	PHE	432	7.778	18.817	76.425	1.00	18.74	
ATOM	1726	CG	PHE	432	8.099	19.713	75.249	1.00	17.54	
ATOM	1727	CD1	PHE	432	8.649	20.976	75.448	1.00	18.72	
ATOM	1728	CD2	PHE	432	7.851	19.290	73.958	1.00	17.78	
ATOM	1729	CE1	PHE	432	8.941	21.800	74.351	1.00	18.20	
ATOM	1730	CE2	PHE	432	8.135	20.093	72.863	1.00	18.04	
ATOM	1731	CZ	PHE	432	8.684	21.358	73.060	1.00	19.15	
ATOM	1732	C	PHE	432	8.817	17.989	78.550	1.00	18.32	
ATOM	1733	O	PHE	432	9.170	18.872	79.330	1.00	20.66	
ATOM	1734	N	GLU	433	8.249	16.852	78.964	1.00	17.15	
ATOM	1735	CA	GLU	433	8.073	16.592	80.382	1.00	20.50	
ATOM	1736	CB	GLU	433	7.520	15.192	80.613	1.00	19.84	
ATOM	1737	CG	GLU	433	6.045	15.053	80.320	1.00	27.71	
ATOM	1738	CD	GLU	433	5.533	13.688	80.744	1.00	31.07	
ATOM	1739	OE1	GLU	433	5.964	13.224	81.823	1.00	34.98	
ATOM	1740	OE2	GLU	433	4.714	13.094	80.006	1.00	34.76	
ATOM	1741	C	GLU	433	9.437	16.691	81.052	1.00	19.32	
ATOM	1742	O	GLU	433	9.574	17.322	82.106	1.00	20.27	
ATOM	1743	N	HIS	434	10.438	16.059	80.435	1.00	18.45	
ATOM	1744	CA	HIS	434	11.810	16.086	80.972	1.00	19.10	
ATOM	1745	CB	HIS	434	12.708	15.091	80.247	1.00	20.67	
ATOM	1746	CG	HIS	434	12.346	13.662	80.495	1.00	21.88	
ATOM	1747	CD2	HIS	434	12.196	12.621	79.642	1.00	22.64	
ATOM	1748	ND1	HIS	434	12.153	13.151	81.763	1.00	24.64	
ATOM	1749	CE1	HIS	434	11.901	11.857	81.678	1.00	26.38	
ATOM	1750	NE2	HIS	434	11.924	11.509	80.403	1.00	25.49	
ATOM	1751	C	HIS	434	12.448	17.471	80.900	1.00	19.47	
ATOM	1752	O	HIS	434	13.029	17.930	81.868	1.00	20.51	
ATOM	1753	N	LEU	435	12.360	18.122	79.749	1.00	17.30	
ATOM	1754	CA	LEU	435	12.926	19.464	79.614	1.00	17.70	

ATOM	1755	CB	LEU	435	12.660	20.017	78.219	1.00	17.54
ATOM	1756	CG	LEU	435	13.350	19.239	77.100	1.00	17.06
ATOM	1757	CD1	LEU	435	12.933	19.793	75.764	1.00	19.34
ATOM	1758	CD2	LEU	435	14.874	19.343	77.242	1.00	19.09
ATOM	1759	C	LEU	435	12.334	20.411	80.653	1.00	17.96
ATOM	1760	O	LEU	435	13.034	21.260	81.193	1.00	18.73
ATOM	1761	N	PHE	436	11.035	20.302	80.921	1.00	17.35
ATOM	1762	CA	PHE	436	10.460	21.192	81.936	1.00	18.85
ATOM	1763	CB	PHE	436	8.920	21.188	81.897	1.00	19.91
ATOM	1764	CG	PHE	436	8.340	21.916	80.720	1.00	22.43
ATOM	1765	CD1	PHE	436	8.885	23.113	80.288	1.00	23.77
ATOM	1766	CD2	PHE	436	7.243	21.399	80.040	1.00	23.20
ATOM	1767	CE1	PHE	436	8.353	23.783	79.202	1.00	25.60
ATOM	1768	CE2	PHE	436	6.703	22.063	78.942	1.00	22.41
ATOM	1769	CZ	PHE	436	7.250	23.249	78.521	1.00	26.06
ATOM	1770	C	PHE	436	10.916	20.802	83.332	1.00	20.10
ATOM	1771	O	PHE	436	11.195	21.670	84.161	1.00	22.89
ATOM	1772	N	PHE	437	11.001	19.500	83.605	1.00	19.98
ATOM	1773	CA	PHE	437	11.412	19.023	84.922	1.00	21.11
ATOM	1774	CB	PHE	437	11.364	17.484	84.974	1.00	21.57
ATOM	1775	CG	PHE	437	11.628	16.913	86.339	1.00	25.91
ATOM	1776	CD1	PHE	437	10.633	16.924	87.313	1.00	27.17
ATOM	1777	CD2	PHE	437	12.881	16.419	86.665	1.00	27.22
ATOM	1778	CE1	PHE	437	10.891	16.447	88.599	1.00	30.66
ATOM	1779	CE2	PHE	437	13.153	15.942	87.944	1.00	31.40
ATOM	1780	CZ	PHE	437	12.158	15.957	88.910	1.00	29.78
ATOM	1781	C	PHE	437	12.807	19.496	85.305	1.00	22.67
ATOM	1782	O	PHE	437	13.046	19.895	86.464	1.00	24.17
ATOM	1783	N	PHE	438	13.724	19.453	84.346	1.00	19.58
ATOM	1784	CA	PHE	438	15.103	19.888	84.567	1.00	22.15
ATOM	1785	CB	PHE	438	16.038	19.027	83.718	1.00	22.90
ATOM	1786	CG	PHE	438	16.093	17.595	84.171	1.00	23.82
ATOM	1787	CD1	PHE	438	16.725	17.262	85.361	1.00	24.00
ATOM	1788	CD2	PHE	438	15.509	16.584	83.419	1.00	27.39
ATOM	1789	CE1	PHE	438	16.773	15.942	85.795	1.00	25.11
ATOM	1790	CE2	PHE	438	15.557	15.253	83.847	1.00	27.37

ATOM 1791 CZ PHE 438 16.188 14.935 85.033 1.00 27.90
ATOM 1792 C PHE 438 15.334 21.383 84.256 1.00 21.04
ATOM 1793 O PHE 438 16.454 21.875 84.352 1.00 22.98
ATOM 1794 N HIS 439 14.267 22.077 83.867 1.00 19.84
ATOM 1795 CA HIS 439 14.311 23.503 83.508 1.00 19.79
ATOM 1796 CB HIS 439 14.550 24.380 84.742 1.00 21.68
ATOM 1797 CG HIS 439 13.463 24.294 85.763 1.00 24.96
ATOM 1798 CD2 HIS 439 12.345 25.037 85.939 1.00 27.66
ATOM 1799 ND1 HIS 439 13.440 23.331 86.747 1.00 26.44
ATOM 1800 CE1 HIS 439 12.353 23.481 87.481 1.00 27.37
ATOM 1801 NE2 HIS 439 11.672 24.511 87.012 1.00 28.08
ATOM 1802 C HIS 439 15.375 23.803 82.469 1.00 20.93
ATOM 1803 O HIS 439 16.185 24.726 82.626 1.00 23.42
ATOM 1804 N LEU 440 15.318 23.068 81.366 1.00 16.51
ATOM 1805 CA LEU 440 16.289 23.200 80.301 1.00 18.97
ATOM 1806 CB LEU 440 16.820 21.813 79.917 1.00 19.31
ATOM 1807 CG LEU 440 17.585 21.101 81.017 1.00 21.82
ATOM 1808 CD1 LEU 440 17.920 19.672 80.567 1.00 24.43
ATOM 1809 CD2 LEU 440 18.839 21.874 81.341 1.00 21.97
ATOM 1810 C LEU 440 15.751 23.859 79.042 1.00 20.05
ATOM 1811 O LEU 440 16.497 24.030 78.099 1.00 21.82
ATOM 1812 N VAL 441 14.478 24.229 79.038 1.00 19.87
ATOM 1813 CA VAL 441 13.879 24.814 77.833 1.00 21.84
ATOM 1814 CB VAL 441 12.795 23.830 77.247 1.00 22.63
ATOM 1815 CG1 VAL 441 11.601 23.713 78.192 1.00 22.79
ATOM 1816 CG2 VAL 441 12.365 24.276 75.855 1.00 24.87
ATOM 1817 C VAL 441 13.306 26.224 78.045 1.00 22.01
ATOM 1818 O VAL 441 12.587 26.478 79.009 1.00 20.37
ATOM 1819 N ALA 442 13.646 27.122 77.120 1.00 23.96
ATOM 1820 CA ALA 442 13.233 28.529 77.172 1.00 27.08
ATOM 1821 CB ALA 442 14.246 29.393 76.392 1.00 28.21
ATOM 1822 C ALA 442 11.846 28.718 76.591 1.00 28.96
ATOM 1823 O ALA 442 11.655 29.494 75.658 1.00 30.12
ATOM 1824 N ASP 443 10.895 28.011 77.178 1.00 30.46
ATOM 1825 CA ASP 443 9.493 27.994 76.764 1.00 31.83
ATOM 1826 CB ASP 443 8.678 27.367 77.906 1.00 33.17

ATOM 1827 CG ASP 443 7.208 27.218 77.581 1.00 34.98
ATOM 1828 OD1 ASP 443 6.856 26.945 76.404 1.00 37.47
ATOM 1829 OD2 ASP 443 6.404 27.346 78.524 1.00 31.58
ATOM 1830 C ASP 443 8.873 29.320 76.318 1.00 31.97
ATOM 1831 O ASP 443 8.426 29.453 75.180 1.00 30.41
ATOM 1832 N THR 444 8.854 30.304 77.205 1.00 32.53
ATOM 1833 CA THR 444 8.236 31.586 76.891 1.00 32.98
ATOM 1834 CB THR 444 7.965 32.371 78.198 1.00 34.53
ATOM 1835 OG1 THR 444 9.196 32.581 78.900 1.00 37.04
ATOM 1836 CG2 THR 444 7.020 31.577 79.102 1.00 35.95
ATOM 1837 C THR 444 8.981 32.486 75.901 1.00 32.99
ATOM 1838 O THR 444 8.399 33.436 75.370 1.00 32.71
ATOM 1839 N SER 445 10.248 32.179 75.639 1.00 30.56
ATOM 1840 CA SER 445 11.071 32.977 74.727 1.00 29.90
ATOM 1841 CB SER 445 12.481 33.132 75.313 1.00 29.52
ATOM 1842 OG SER 445 12.418 33.766 76.576 1.00 31.76
ATOM 1843 C SER 445 11.199 32.429 73.308 1.00 29.39
ATOM 1844 O SER 445 11.580 33.153 72.387 1.00 28.30
ATOM 1845 N ILE 446 10.875 31.151 73.133 1.00 26.98
ATOM 1846 CA ILE 446 11.010 30.511 71.840 1.00 25.95
ATOM 1847 CB ILE 446 10.656 29.013 71.961 1.00 26.36
ATOM 1848 CG2 ILE 446 10.295 28.431 70.595 1.00 24.39
ATOM 1849 CG1 ILE 446 11.864 28.300 72.575 1.00 27.57
ATOM 1850 CD1 ILE 446 11.637 26.869 72.971 1.00 27.13
ATOM 1851 C ILE 446 10.312 31.144 70.640 1.00 25.28
ATOM 1852 O ILE 446 10.917 31.247 69.571 1.00 23.47
ATOM 1853 N ALA 447 9.058 31.549 70.809 1.00 26.37
ATOM 1854 CA ALA 447 8.316 32.183 69.725 1.00 28.80
ATOM 1855 CB ALA 447 6.932 32.606 70.219 1.00 30.52
ATOM 1856 C ALA 447 9.114 33.394 69.218 1.00 28.51
ATOM 1857 O ALA 447 9.229 33.608 68.005 1.00 29.41
ATOM 1858 N GLY 448 9.675 34.164 70.155 1.00 28.53
ATOM 1859 CA GLY 448 10.474 35.337 69.811 1.00 27.89
ATOM 1860 C GLY 448 11.762 34.993 69.095 1.00 28.77
ATOM 1861 O GLY 448 12.167 35.692 68.162 1.00 28.23
ATOM 1862 N TYR 449 12.435 33.927 69.536 1.00 27.26

ATOM	1863	CA	TYR	449	13.666	33.502	68.872	1.00	28.14
ATOM	1864	CB	TYR	449	14.262	32.267	69.553	1.00	26.16
ATOM	1865	CG	TYR	449	14.683	32.492	70.990	1.00	28.82
ATOM	1866	CD1	TYR	449	14.913	33.782	71.482	1.00	29.84
ATOM	1867	CE1	TYR	449	15.336	33.988	72.802	1.00	32.66
ATOM	1868	CD2	TYR	449	14.881	31.412	71.853	1.00	29.90
ATOM	1869	CE2	TYR	449	15.306	31.604	73.173	1.00	30.71
ATOM	1870	CZ	TYR	449	15.532	32.887	73.641	1.00	32.74
ATOM	1871	OH	TYR	449	15.979	33.070	74.939	1.00	36.98
ATOM	1872	C	TYR	449	13.361	33.150	67.420	1.00	27.51
ATOM	1873	O	TYR	449	14.116	33.491	66.513	1.00	27.99
ATOM	1874	N	ILE	450	12.254	32.442	67.207	1.00	27.41
ATOM	1875	CA	ILE	450	11.876	32.053	65.861	1.00	27.70
ATOM	1876	CB	ILE	450	10.662	31.102	65.863	1.00	26.64
ATOM	1877	CG2	ILE	450	10.292	30.744	64.413	1.00	26.88
ATOM	1878	CG1	ILE	450	11.003	29.846	66.690	1.00	27.46
ATOM	1879	CD1	ILE	450	9.811	28.956	67.032	1.00	24.45
ATOM	1880	C	ILE	450	11.534	33.295	65.041	1.00	29.34
ATOM	1881	O	ILE	450	11.994	33.440	63.911	1.00	30.32
ATOM	1882	N	ARG	451	10.735	34.187	65.617	1.00	30.43
ATOM	1883	CA	ARG	451	10.351	35.416	64.923	1.00	33.00
ATOM	1884	CB	ARG	451	9.514	36.306	65.851	1.00	32.56
ATOM	1885	CG	ARG	451	8.874	37.519	65.161	1.00	34.91
ATOM	1886	CD	ARG	451	7.955	38.328	66.076	1.00	36.14
ATOM	1887	NE	ARG	451	6.768	37.599	66.518	1.00	37.46
ATOM	1888	CZ	ARG	451	6.669	36.943	67.672	1.00	40.02
ATOM	1889	NH1	ARG	451	7.690	36.921	68.521	1.00	41.16
ATOM	1890	NH2	ARG	451	5.547	36.299	67.976	1.00	40.59
ATOM	1891	C	ARG	451	11.629	36.138	64.472	1.00	34.57
ATOM	1892	O	ARG	451	11.761	36.516	63.298	1.00	34.59
ATOM	1893	N	ASP	452	12.578	36.304	65.392	1.00	36.05
ATOM	1894	CA	ASP	452	13.837	36.975	65.070	1.00	39.88
ATOM	1895	CB	ASP	452	14.690	37.184	66.331	1.00	42.41
ATOM	1896	CG	ASP	452	14.004	38.065	67.364	1.00	46.01
ATOM	1897	OD1	ASP	452	13.162	38.897	66.961	1.00	46.57
ATOM	1898	OD2	ASP	452	14.315	37.934	68.576	1.00	48.55

ATOM	1899	C	ASP	452	14.657	36.212	64.039	1.00	40.80
ATOM	1900	O	ASP	452	15.219	36.805	63.112	1.00	42.52
ATOM	1901	N	ALA	453	14.730	34.896	64.197	1.00	41.16
ATOM	1902	CA	ALA	453	15.493	34.071	63.272	1.00	42.41
ATOM	1903	CB	ALA	453	15.585	32.643	63.796	1.00	41.71
ATOM	1904	C	ALA	453	14.904	34.070	61.863	1.00	44.06
ATOM	1905	O	ALA	453	15.635	33.910	60.887	1.00	44.96
ATOM	1906	N	LEU	454	13.590	34.259	61.759	1.00	45.34
ATOM	1907	CA	LEU	454	12.921	34.261	60.460	1.00	47.12
ATOM	1908	CB	LEU	454	11.419	33.989	60.631	1.00	42.61
ATOM	1909	CG	LEU	454	11.078	32.514	60.884	1.00	38.89
ATOM	1910	CD1	LEU	454	9.576	32.329	60.950	1.00	36.29
ATOM	1911	CD2	LEU	454	11.660	31.657	59.764	1.00	36.23
ATOM	1912	C	LEU	454	13.149	35.544	59.669	1.00	50.37
ATOM	1913	O	LEU	454	13.255	35.506	58.443	1.00	51.61
ATOM	1914	N	ARG	455	13.218	36.679	60.360	1.00	54.48
ATOM	1915	CA	ARG	455	13.486	37.951	59.688	1.00	58.31
ATOM	1916	CB	ARG	455	13.128	39.147	60.582	1.00	59.22
ATOM	1917	CG	ARG	455	11.635	39.352	60.806	1.00	60.97
ATOM	1918	CD	ARG	455	11.318	40.787	61.228	1.00	62.50
ATOM	1919	NE	ARG	455	10.998	40.919	62.648	1.00	64.04
ATOM	1920	CZ	ARG	455	11.873	40.784	63.640	1.00	64.71
ATOM	1921	NH1	ARG	455	13.146	40.511	63.378	1.00	64.92
ATOM	1922	NH2	ARG	455	11.470	40.923	64.897	1.00	64.48
ATOM	1923	C	ARG	455	14.988	37.938	59.452	1.00	60.72
ATOM	1924	O	ARG	455	15.597	38.964	59.147	1.00	61.55
ATOM	1925	N	ASN	456	15.557	36.743	59.597	1.00	63.01
ATOM	1926	CA	ASN	456	16.983	36.482	59.463	1.00	64.82
ATOM	1927	CB	ASN	456	17.434	36.512	57.987	1.00	66.21
ATOM	1928	CG	ASN	456	17.254	37.871	57.327	1.00	67.51
ATOM	1929	OD1	ASN	456	17.901	38.850	57.702	1.00	68.69
ATOM	1930	ND2	ASN	456	16.377	37.930	56.326	1.00	68.01
ATOM	1931	C	ASN	456	17.795	37.442	60.317	1.00	65.37
ATOM	1932	O	ASN	456	17.456	37.680	61.480	1.00	65.63
ATOM	1933	N	GLY	457	18.858	37.997	59.749	1.00	65.99
ATOM	1934	CA	GLY	457	19.704	38.896	60.510	1.00	66.46

ATOM	1935	C	GLY	457	20.739	38.015	61.176	1.00	66.78
ATOM	1936	O	GLY	457	21.568	38.471	61.968	1.00	67.21
ATOM	1937	N	GLY	458	20.669	36.728	60.844	1.00	66.86
ATOM	1938	CA	GLY	458	21.594	35.753	61.384	1.00	66.84
ATOM	1939	C	GLY	458	22.018	34.761	60.315	1.00	66.86
ATOM	1940	O	GLY	458	21.450	34.801	59.199	1.00	66.65
ATOM	1941	OXT	GLY	458	22.922	33.943	60.593	1.00	65.49
ATOM	1942	OH2	TIP	1003	30.252	23.128	74.386	1.00	27.69
ATOM	1943	OH2	TIP	1005	14.203	25.558	89.644	1.00	25.22
ATOM	1944	OH2	TIP	1006	8.388	25.042	72.262	1.00	22.81
ATOM	1945	OH2	TIP	1008	8.367	21.538	69.460	1.00	19.23
ATOM	1946	OH2	TIP	1009	-7.350	22.030	52.884	1.00	80.11
ATOM	1947	OH2	TIP	1010	-4.017	19.644	67.897	1.00	33.26
ATOM	1948	OH2	TIP	1011	8.365	3.022	77.974	1.00	47.93
ATOM	1949	OH2	TIP	1012	30.690	8.779	67.839	1.00	26.30
ATOM	1950	OH2	TIP	1013	12.264	8.843	80.249	1.00	26.01
ATOM	1951	OH2	TIP	1014	-1.764	16.382	62.652	1.00	44.82
ATOM	1952	OH2	TIP	1015	20.301	34.946	75.498	1.00	51.92
ATOM	1953	OH2	TIP	1016	14.443	15.693	61.296	1.00	22.04
ATOM	1954	OH2	TIP	1017	12.487	31.635	78.951	1.00	36.76
ATOM	1955	OH2	TIP	1018	16.579	6.557	83.739	1.00	27.86
ATOM	1956	OH2	TIP	1019	-0.626	26.615	50.499	1.00	30.82
ATOM	1957	OH2	TIP	1021	3.543	20.127	64.859	1.00	23.80
ATOM	1958	OH2	TIP	1022	4.772	0.996	47.855	1.00	40.67
ATOM	1959	OH2	TIP	1023	9.799	29.451	51.621	1.00	30.93
ATOM	1960	OH2	TIP	1024	7.476	19.030	68.589	1.00	22.30
ATOM	1961	OH2	TIP	1025	20.355	7.131	58.551	1.00	52.44
ATOM	1962	OH2	TIP	1026	-0.829	29.526	57.153	1.00	31.90
ATOM	1963	OH2	TIP	1027	11.560	-6.342	53.442	1.00	52.29
ATOM	1964	OH2	TIP	1028	15.278	0.625	72.808	1.00	27.12
ATOM	1965	OH2	TIP	1029	22.593	26.832	76.012	1.00	35.56
ATOM	1966	OH2	TIP	1031	3.001	25.878	68.078	1.00	22.76
ATOM	1967	OH2	TIP	1032	13.489	25.800	47.958	1.00	47.50
ATOM	1968	OH2	TIP	1033	-7.554	18.088	60.905	1.00	30.53
ATOM	1969	OH2	TIP	1034	24.742	18.595	64.446	1.00	44.88
ATOM	1970	OH2	TIP	1035	13.751	37.059	78.800	1.00	60.77

ATOM 1971 OH2 TIP 1036 -0.515 10.167 75.163 1.00 36.51
ATOM 1972 OH2 TIP 1037 12.373 35.911 72.901 1.00 32.65
ATOM 1973 OH2 TIP 1039 23.543 26.270 78.523 1.00 24.40
ATOM 1974 OH2 TIP 1040 17.896 20.961 59.259 1.00 39.57
ATOM 1975 OH2 TIP 1041 8.248 15.187 89.930 1.00 59.85
ATOM 1976 OH2 TIP 1042 7.418 31.128 73.133 1.00 34.33
ATOM 1977 OH2 TIP 1043 21.123 8.890 53.894 1.00 67.39
ATOM 1978 OH2 TIP 1045 15.162 18.243 53.355 1.00 28.26
ATOM 1979 OH2 TIP 1050 4.216 23.224 44.827 1.00 46.56
ATOM 1980 OH2 TIP 1051 17.523 1.262 73.909 1.00 23.12
ATOM 1981 OH2 TIP 1052 -0.169 20.149 67.166 1.00 67.45
ATOM 1982 OH2 TIP 1053 20.135 12.837 55.866 1.00 51.70
ATOM 1983 OH2 TIP 1054 10.612 35.387 77.215 1.00 57.20
ATOM 1984 OH2 TIP 1055 14.587 38.805 73.912 1.00 56.14
ATOM 1985 OH2 TIP 1056 22.658 15.094 55.769 1.00 63.46
ATOM 1986 OH2 TIP 1057 8.196 1.415 39.058 1.00 55.65
ATOM 1987 OH2 TIP 1058 10.807 2.725 77.173 1.00 22.15
ATOM 1988 OH2 TIP 1059 19.013 20.604 62.130 1.00 32.43
ATOM 1989 OH2 TIP 1061 2.388 16.861 45.084 1.00 25.70
ATOM 1990 OH2 TIP 1063 5.229 6.816 86.424 1.00 59.99
ATOM 1991 OH2 TIP 1501 18.919 15.965 66.146 1.00 24.36
ATOM 1992 OH2 TIP 1502 2.744 33.258 66.246 1.00 30.10
ATOM 1993 OH2 TIP 1503 4.527 17.244 77.877 1.00 23.98
ATOM 1994 OH2 TIP 1504 -0.815 22.723 68.903 1.00 24.06
ATOM 1995 OH2 TIP 1506 22.697 1.204 69.760 1.00 28.71
ATOM 1996 OH2 TIP 1507 12.438 25.185 81.547 1.00 28.20
ATOM 1997 OH2 TIP 1508 17.107 31.275 76.636 1.00 33.34
ATOM 1998 OH2 TIP 1509 17.900 15.686 59.270 1.00 37.88
ATOM 1999 OH2 TIP 1510 7.197 12.183 44.002 1.00 29.62
ATOM 2000 OH2 TIP 1511 -4.834 15.832 60.463 1.00 33.76
ATOM 2001 OH2 TIP 1512 11.093 1.186 74.736 1.00 29.08
ATOM 2002 OH2 TIP 1513 -0.145 2.568 51.845 1.00 30.78
ATOM 2003 OH2 TIP 1514 -6.100 23.488 73.541 1.00 27.96
ATOM 2004 OH2 TIP 1515 8.298 14.512 44.198 1.00 34.89
ATOM 2005 OH2 TIP 1516 0.418 26.098 68.989 1.00 28.71
ATOM 2006 OH2 TIP 1517 -7.177 16.116 59.030 1.00 32.04

ATOM	2007	OH2	TIP	1519	18.000	18.387	62.314	1.00	32.49
ATOM	2008	OH2	TIP	1520	21.777	20.403	61.898	1.00	38.66
ATOM	2009	OH2	TIP	1521	-1.379	32.714	63.883	1.00	40.86
ATOM	2010	OH2	TIP	1522	1.931	22.610	68.721	1.00	31.49
ATOM	2011	OH2	TIP	1523	-3.158	9.157	64.790	1.00	46.08
ATOM	2012	OH2	TIP	1524	2.081	4.709	65.432	1.00	38.87
ATOM	2013	OH2	TIP	1525	3.829	11.325	75.940	1.00	34.36
ATOM	2014	OH2	TIP	1527	21.845	33.747	71.839	1.00	51.86
ATOM	2015	OH2	TIP	1528	12.196	0.941	78.760	1.00	46.53
ATOM	2016	OH2	TIP	1529	30.316	21.478	85.009	1.00	28.49
ATOM	2017	OH2	TIP	1530	9.786	2.798	91.182	1.00	58.36
ATOM	2018	OH2	TIP	1531	16.571	8.007	48.772	1.00	38.32
ATOM	2019	OH2	TIP	1532	3.764	24.595	70.409	1.00	31.40
ATOM	2020	OH2	TIP	1533	-0.952	5.111	57.996	1.00	39.42
ATOM	2021	OH2	TIP	1534	8.395	29.793	48.733	1.00	45.92
ATOM	2022	OH2	TIP	1535	18.190	-0.943	54.382	1.00	55.57
ATOM	2023	OH2	TIP	1536	4.583	13.859	64.203	1.00	30.44
ATOM	2024	OH2	TIP	1538	12.012	14.232	84.365	1.00	33.97
ATOM	2025	OH2	TIP	1539	-1.284	36.017	69.736	1.00	57.91
ATOM	2026	OH2	TIP	1540	2.454	15.898	79.022	1.00	40.22
ATOM	2027	OH2	TIP	1544	2.719	2.670	49.088	1.00	32.00
ATOM	2028	OH2	TIP	1545	13.537	37.410	71.136	1.00	41.29
ATOM	2029	OH2	TIP	1546	22.697	0.071	79.248	1.00	32.01
ATOM	2030	OH2	TIP	1548	-0.239	7.542	39.851	1.00	52.37
ATOM	2031	OH2	TIP	1549	0.076	10.603	44.453	1.00	41.67
ATOM	2032	OH2	TIP	1550	31.157	3.039	59.611	1.00	43.66
ATOM	2033	OH2	TIP	1551	4.226	34.045	72.549	1.00	53.58
ATOM	2034	OH2	TIP	1554	10.022	33.359	56.088	1.00	41.48
ATOM	2035	OH2	TIP	1555	-1.058	37.708	61.917	1.00	54.81
ATOM	2036	OH2	TIP	1556	-4.583	15.870	53.480	1.00	37.02
ATOM	2037	OH2	TIP	1557	23.851	8.517	92.595	1.00	36.91
ATOM	2038	OH2	TIP	1558	-7.204	28.744	59.955	1.00	35.72
ATOM	2039	OH2	TIP	1560	19.483	16.334	88.331	1.00	34.61
ATOM	2040	OH2	TIP	1561	1.968	8.086	38.648	1.00	57.90
ATOM	2041	OH2	TIP	1562	32.430	-4.459	71.625	1.00	63.22
ATOM	2042	OH2	TIP	1563	7.819	12.682	83.368	1.00	47.71

ATOM	2043	OH2	TIP	1564	-5.435	18.376	72.810	1.00	41.90
ATOM	2044	OH2	TIP	1565	19.550	17.394	63.917	1.00	31.79
ATOM	2045	OH2	TIP	1566	24.069	28.502	85.703	1.00	50.24
ATOM	2046	OH2	TIP	1568	26.854	12.830	56.392	1.00	51.68
ATOM	2047	OH2	TIP	1570	3.595	32.325	68.760	1.00	45.07
ATOM	2048	OH2	TIP	1571	24.805	8.300	62.036	1.00	28.27
ATOM	2049	OH2	TIP	1572	4.194	17.554	63.640	1.00	26.21
ATOM	2050	OH2	TIP	1573	2.589	20.195	67.352	1.00	34.52
ATOM	2051	OH2	TIP	1574	15.713	17.937	61.017	1.00	52.03
ATOM	2052	OH2	TIP	1575	-9.321	14.210	59.772	1.00	33.92
ATOM	2053	OH2	TIP	1576	13.215	7.332	82.542	1.00	31.45
ATOM	2054	OH2	TIP	1577	10.470	24.539	83.194	1.00	35.29
ATOM	2055	OH2	TIP	1578	25.712	17.999	53.496	1.00	41.46
ATOM	2056	OH2	TIP	1579	9.445	-0.239	41.882	1.00	41.51
ATOM	2057	OH2	TIP	1580	6.603	16.005	42.611	1.00	32.35
ATOM	2058	OH2	TIP	1581	-1.523	7.654	59.739	1.00	50.11
ATOM	2059	OH2	TIP	1582	8.397	34.515	72.891	1.00	33.81
ATOM	2060	OH2	TIP	1583	2.742	39.191	60.949	1.00	39.77
ATOM	2061	OH2	TIP	1584	18.933	6.009	52.002	1.00	45.27
ATOM	2062	OH2	TIP	1585	-1.653	20.171	69.665	1.00	37.15
ATOM	2063	OH2	TIP	1586	-2.633	4.655	52.475	1.00	49.05
ATOM	2064	OH2	TIP	1587	36.297	28.180	83.444	1.00	41.56
ATOM	2065	OH2	TIP	1588	-0.851	31.806	55.808	1.00	34.41
ATOM	2066	OH2	TIP	1589	4.002	34.625	70.007	1.00	46.13
ATOM	2067	OH2	TIP	1590	32.711	20.152	84.581	1.00	53.56
ATOM	2068	OH2	TIP	1591	19.998	6.099	87.630	1.00	31.12
ATOM	2069	OH2	TIP	1593	-0.189	3.637	35.682	1.00	54.58
ATOM	2070	OH2	TIP	1594	12.455	12.705	39.358	1.00	55.12
ATOM	2071	OH2	TIP	1596	-2.554	-6.074	47.925	1.00	55.01
ATOM	2072	OH2	TIP	1597	5.017	28.176	75.017	1.00	42.02
ATOM	2073	OH2	TIP	1598	28.617	32.433	80.891	1.00	65.40
ATOM	2074	OH2	TIP	1599	8.680	7.258	78.481	1.00	52.56
ATOM	2075	OH2	TIP	1600	18.188	12.950	87.437	1.00	47.03
ATOM	2076	OH2	TIP	1601	-11.532	19.931	55.756	1.00	48.92
ATOM	2077	OH2	TIP	1602	22.073	14.215	52.571	1.00	49.32
ATOM	2078	OH2	TIP	1603	-3.860	34.262	53.170	1.00	48.97

ATOM	2079	OH2	TIP	1604	1.118	10.847	82.180	1.00 44.11
ATOM	2080	OH2	TIP	1605	19.335	32.031	77.782	1.00 48.61
ATOM	2081	OH2	TIP	1606	19.174	9.955	48.654	1.00 40.42
ATOM	2082	OH2	TIP	1607	23.632	-1.631	71.300	1.00 37.97
ATOM	2083	OH2	TIP	1608	26.622	26.695	85.361	1.00 44.14
ATOM	2084	OH2	TIP	1609	22.586	-1.769	57.526	1.00 48.15
ATOM	2085	OH2	TIP	1610	21.977	5.567	60.712	1.00 37.76
ATOM	2086	OH2	TIP	1611	21.634	2.725	67.903	1.00 41.42
ATOM	2087	OH2	TIP	1612	4.046	4.187	75.513	1.00 55.86
ATOM	2088	OH2	TIP	1614	0.807	25.979	47.960	1.00 38.30
ATOM	2089	OH2	TIP	1615	17.333	37.351	72.160	1.00 55.70
ATOM	2090	OH2	TIP	1616	2.475	15.902	62.566	1.00 38.40
ATOM	2091	OH2	TIP	1618	0.658	14.983	64.592	1.00 60.57
ATOM	2092	OH2	TIP	1619	-6.509	17.844	52.643	1.00 41.17
ATOM	2093	OH2	TIP	1621	27.000	-1.287	80.946	1.00 51.49
ATOM	2094	OH2	TIP	1622	3.271	9.154	86.392	1.00 55.17
ATOM	2095	OH2	TIP	1627	3.433	19.409	44.225	1.00 50.54
ATOM	2096	OH2	TIP	1628	2.390	26.629	72.360	1.00 42.60
ATOM	2097	OH2	TIP	1629	9.893	39.104	69.833	1.00 54.40
ATOM	2098	OH2	TIP	1630	2.709	14.153	43.455	1.00 34.37
ATOM	2099	OH2	TIP	1631	11.049	12.448	88.232	1.00 45.81
ATOM	2100	OH2	TIP	1632	4.576	31.506	72.757	1.00 39.34
ATOM	2101	OH2	TIP	1634	6.784	36.285	71.148	1.00 51.53
ATOM	2102	OH2	TIP	1635	6.667	43.335	56.568	1.00 51.21
ATOM	2103	OH2	TIP	1636	-5.771	9.260	60.442	1.00 44.79
ATOM	2104	OH2	TIP	1638	0.052	33.418	66.937	1.00 47.03
ATOM	2105	OH2	TIP	1641	0.354	1.055	46.133	1.00 54.03
ATOM	2106	OH2	TIP	1642	24.406	30.113	88.300	1.00 48.82
ATOM	2107	OH2	TIP	1643	26.619	20.182	66.495	1.00 38.01
ATOM	2108	OH2	TIP	1644	17.492	7.024	42.815	1.00 65.02
ATOM	2109	OH2	TIP	1645	25.942	26.481	82.676	1.00 49.52
ATOM	2110	OH2	TIP	1646	20.601	16.199	68.672	1.00 37.35
ATOM	2111	OH2	TIP	1649	27.616	9.156	63.460	1.00 37.92
ATOM	2112	OH2	TIP	1650	0.428	-3.038	44.190	1.00 54.50
ATOM	2113	OH2	TIP	1652	-7.028	20.462	59.299	1.00 33.58
ATOM	2114	OH2	TIP	1653	-2.848	32.314	67.354	1.00 49.02

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ATOM  2115 OH2 TIP  1654     -0.686  17.762  66.362  1.00 46.03
ATOM  2116 OH2 TIP  1655     19.583  17.275  60.162  1.00 41.00
ATOM  2117 OH2 TIP  1656     13.719  36.618  75.139  1.00 51.89
ATOM  2118 OH2 TIP  1657      9.386  -0.422  71.399  1.00 43.15
ATOM  2119 OH2 TIP  1659     23.690  28.880  79.578  1.00 42.62
ATOM  2120 OH2 TIP  1660     22.069   3.800  58.682  1.00 46.06
ATOM  2121 OH2 TIP  1661     20.671  13.353  58.841  1.00 57.05
ATOM  2122 OH2 TIP  1662     27.473  10.135  82.332  1.00 47.43
ATOM  2123 OH2 TIP  1664      9.564  26.542  84.601  1.00 44.55
ATOM  2124 OH2 TIP  1666     29.122   9.606  65.764  1.00 45.20
ATOM  2125 OH2 TIP  1668     13.135  20.507  41.865  1.00 59.09
ATOM  2126 OH2 TIP  1669     22.639  11.672  58.999  1.00 54.98
ATOM  2127 OH2 TIP  1670     -1.845   6.027  76.197  1.00 48.89
ATOM  2128 OH2 TIP  1672      4.883  25.252  42.734  1.00 51.13
ATOM  2129 OH2 TIP  1675      1.329  39.322  66.763  1.00 68.30
ATOM  2130 OH2 TIP  1676     12.783  29.313  87.079  1.00 54.62
ATOM  2131 OH2 TIP  1679     25.035  18.339  57.364  1.00 54.53
ATOM  2132 OH2 TIP  1682     29.392  -1.856  57.721  1.00 37.30
ATOM  2133 OH2 TIP  1683     28.780   9.970  58.622  1.00 54.22
ATOM  2134 OH2 TIP  1685      4.741  39.274  62.499  1.00 46.58
ATOM  2135 OH2 TIP  1686     -3.084   6.977  49.478  1.00 57.17
ATOM  2136 OH2 TIP  1687     26.519  30.868  83.197  1.00 64.53
ATOM  2137 OH2 TIP  1688     -2.784  37.278  67.289  1.00 59.53
ATOM  2138 OH2 TIP  1689     18.691  10.604  88.296  1.00 52.44
ATOM  2139 OH2 TIP  1690     27.919   6.703  82.226  1.00 44.84
ATOM  2140 OH2 TIP  1691     -4.338  11.103  48.033  1.00 55.91
ATOM  2141 OH2 TIP  1692     -7.853   9.429  46.864  1.00 63.74
ATOM  2142 OH2 TIP  1693     10.901  -1.686  67.477  1.00 41.21
ATOM  2143 OH2 TIP  1694     -2.114   6.315  55.259  1.00 56.21
ATOM  2144 OH2 TIP  1695     17.482  15.932  44.391  1.00 41.18
ATOM  2145 OH2 TIP  1696    -12.326  38.088  61.786  1.00 53.30
ATOM  2146 OH2 TIP  1697     -2.176  40.471  68.230  1.00 68.88
ATOM  2147 OH2 TIP  1700      6.514  -1.974  53.366  1.00 51.67
ATOM  2148 OH2 TIP  1701     21.800  10.610  55.773  1.00 60.93
ATOM  2149 OH2 TIP  1702      3.975  27.046  41.446  1.00 44.88
ATOM  2150 OH2 TIP  1703     26.678  -3.660  64.081  1.00 62.42
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ATOM 2151 OH2 TIP 1704 2.958 12.027 86.133 1.00 53.52
ATOM 2152 OH2 TIP 1705 4.264 22.050 63.018 1.00 16.96
ATOM 2153 OH2 TIP 1706 22.999 26.329 63.006 1.00 32.17
ATOM 2154 OH2 TIP 1707 5.614 2.688 68.201 1.00 42.08
ATOM 2155 OH2 TIP 1708 -2.967 17.730 54.394 1.00 38.89
ATOM 2156 OH2 TIP 1709 25.853 10.594 62.118 1.00 43.50
ATOM 2157 OH2 TIP 1711 13.060 12.966 86.563 1.00 41.22
ATOM 2158 OH2 TIP 1712 19.784 15.472 45.489 1.00 58.17
ATOM 2159 OH2 TIP 1713 10.567 14.806 42.991 1.00 43.48
ATOM 2160 OH2 TIP 1714 24.079 30.190 83.477 1.00 47.61
ATOM 2161 OH2 TIP 1715 23.927 21.975 63.464 1.00 44.77
ATOM 2162 OH2 TIP 1716 15.801 20.193 58.769 1.00 34.32
ATOM 2163 OH2 TIP 1717 23.867 27.717 72.712 1.00 40.47
ATOM 2164 OH2 TIP 1718 24.567 27.201 69.884 1.00 45.97
ATOM 2165 OH2 TIP 1719 32.141 -1.375 73.278 1.00 62.31
ATOM 2166 OH2 TIP 1720 19.799 24.122 57.454 1.00 35.07
ATOM 2167 OH2 TIP 1721 18.297 23.286 53.598 1.00 43.88
ATOM 2168 OH2 TIP 1722 8.617 1.105 73.470 1.00 48.55
ATOM 2169 OH2 TIP 1723 28.598 25.728 64.296 1.00 46.24
ATOM 2170 OH2 TIP 1725 19.225 33.547 73.276 1.00 44.07
ATOM 2171 OH2 TIP 1726 1.762 4.546 47.584 1.00 50.27
ATOM 2172 OH2 TIP 1727 10.895 28.774 83.657 1.00 54.87
ATOM 2173 OH2 TIP 1728 9.989 36.628 73.713 1.00 46.56
ATOM 2174 OH2 TIP 1729 -1.331 8.332 70.133 1.00 46.76
ATOM 2175 OH2 TIP 1730 24.262 12.802 55.386 1.00 59.24
ATOM 2176 OH2 TIP 1731 28.623 25.788 86.798 1.00 51.87
ATOM 2177 OH2 TIP 1732 -0.501 4.843 68.521 1.00 47.96
ATOM 2178 OH2 TIP 1736 18.422 4.635 54.793 1.00 51.00
ATOM 2179 OH2 TIP 1737 -5.388 27.319 50.727 1.00 46.53
ATOM 2180 OH2 TIP 1738 -2.286 20.842 72.915 1.00 45.95
ATOM 2181 OH2 TIP 1739 0.996 4.268 39.511 1.00 52.67
ATOM 2182 OH2 TIP 1740 -10.886 28.616 64.116 1.00 45.22
ATOM 2183 OH2 TIP 1741 20.353 -4.883 70.512 1.00 61.31
ATOM 2184 OH2 TIP 1742 22.491 16.164 60.365 1.00 58.19
ATOM 2185 OH2 TIP 3001 15.272 21.419 87.789 1.00 27.44
ATOM 2186 OH2 TIP 3002 13.055 32.876 52.925 1.00 53.35

ATOM	2187	OH2	TIP	3006	16.014	18.841	64.083	1.00	56.45
ATOM	2188	OH2	TIP	3008	16.802	30.100	54.388	1.00	48.87
ATOM	2189	OH2	TIP	3009	13.673	27.099	82.740	1.00	32.07
ATOM	2190	OH2	TIP	3010	30.041	24.325	84.969	1.00	41.40
ATOM	2191	OH2	TIP	3007	-2.102	35.612	60.958	1.00	52.05
ATOM	2192	OH2	TIP	3011	7.242	14.501	40.017	1.00	51.46
ATOM	2193	OH2	TIP	3012	1.031	36.834	60.593	1.00	49.05
ATOM	2194	OH2	TIP	3013	0.026	24.244	72.355	1.00	42.35
ATOM	2195	OH2	TIP	3015	-7.871	31.986	57.037	1.00	46.09
ATOM	2196	OH2	TIP	3019	8.655	-3.490	62.423	1.00	44.56
ATOM	2197	OH2	TIP	3020	-0.191	30.553	51.677	1.00	54.31
ATOM	2198	OH2	TIP	3023	3.107	37.905	57.599	1.00	48.07
ATOM	2199	OH2	TIP	3024	26.217	6.182	84.277	1.00	47.75
ATOM	2200	OH2	TIP	3025	2.594	16.520	65.838	1.00	40.67
ATOM	2201	C1	EPH	4000	23.874	12.843	85.264	1.00	42.79
ATOM	2202	C2	EPH	4000	23.099	13.772	86.129	1.00	44.39
ATOM	2203	C4	EPH	4000	24.923	13.000	83.062	1.00	45.55
ATOM	2204	O2	EPH	4000	24.221	13.543	84.059	1.00	44.96
ATOM	2205	O4	EPH	4000	25.350	11.876	83.028	1.00	47.53
ATOM	2206	C18	EPH	4000	25.126	14.045	81.931	1.00	47.05
ATOM	2207	C19	EPH	4000	24.674	13.569	80.547	1.00	46.98
ATOM	2208	C20	EPH	4000	23.168	13.412	80.473	1.00	49.00
ATOM	2209	C21	EPH	4000	22.772	12.939	79.111	1.00	51.06
ATOM	2210	C22	EPH	4000	21.365	12.327	79.073	1.00	52.88
ATOM	2211	C23	EPH	4000	20.291	13.230	78.423	1.00	54.24
ATOM	2212	C24	EPH	4000	20.651	13.777	77.022	1.00	55.08
ATOM	2213	C25	EPH	4000	19.987	15.129	76.704	1.00	56.13
ATOM	2214	C26	EPH	4000	20.807	16.375	77.147	1.00	56.19
ATOM	2215	C27	EPH	4000	19.981	17.687	77.287	1.00	56.74
ATOM	2216	C28	EPH	4000	19.188	18.077	76.015	1.00	56.93
ATOM	2217	C29	EPH	4000	20.055	18.393	74.792	1.00	57.07
ATOM	2218	C30	EPH	4000	19.294	18.387	73.442	1.00	58.24
ATOM	2219	C31	EPH	4000	19.391	17.124	72.550	1.00	58.70
ATOM	2220	C32	EPH	4000	18.019	16.479	72.198	1.00	59.07
ATOM	2221	C33	EPH	4000	16.762	17.158	72.768	1.00	59.61
ATOM	2222	C34	EPH	4000	15.463	16.541	72.231	1.00	60.17

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ATOM  2223 C37 EPH 4000     22.780  13.059  87.421  1.00 47.03
ATOM  2224 O5  EPH 4000     22.047  13.939  88.273  1.00 53.23
ATOM  2225 P1  EPH 4000     21.699  13.222  89.578  1.00 56.71
ATOM  2226 O6  EPH 4000     20.350  13.536  89.939  1.00 58.07
ATOM  2227 O7  EPH 4000     22.579  12.360  90.311  1.00 56.72
ATOM  2228 O8  EPH 4000     22.167  14.340  90.336  1.00 55.93
ATOM  2229 C3  EPH 4000     21.561  15.394  85.253  1.00 42.20
ATOM  2230 O1  EPH 4000     21.886  14.117  85.454  1.00 40.69
ATOM  2231 O3  EPH 4000     22.221  16.347  85.571  1.00 40.97
ATOM  2232 C5  EPH 4000     20.215  15.530  84.546  1.00 40.77
ATOM  2233 C6  EPH 4000     20.313  15.776  83.050  1.00 42.19
ATOM  2234 C7  EPH 4000     18.924  15.916  82.453  1.00 43.05
ATOM  2235 C8  EPH 4000     18.900  15.944  80.947  1.00 44.57
ATOM  2236 C9  EPH 4000     17.477  16.101  80.445  1.00 45.49
ATOM  2237 C10 EPH 4000     17.167  15.209  79.273  1.00 47.18
ATOM  2238 C11 EPH 4000     16.561  15.987  78.117  1.00 47.85
ATOM  2239 C12 EPH 4000     15.158  15.514  77.781  1.00 49.75
ATOM  2240 C13 EPH 4000     15.158  14.254  76.932  1.00 49.27
ATOM  2241 C14 EPH 4000     14.899  14.563  75.454  1.00 51.41
ATOM  2242 C15 EPH 4000     14.958  13.341  74.490  1.00 51.93
ATOM  2243 C16 EPH 4000     16.376  12.870  74.074  1.00 52.39
ATOM  2244 C17 EPH 4000     16.681  11.465  74.554  1.00 52.37
ATOM  2245 C35 EPH 4000     17.830  11.518  75.525  1.00 52.96
ATOM  2246 C36 EPH 4000     17.968  10.168  76.193  1.00 53.00
ATOM  2247 C38 EPH 4000     22.197  10.885  90.057  1.00 56.75
ATOM  2248 C39 EPH 4000     23.458  10.026  89.911  1.00 56.42
ATOM  2249 N1  EPH 4000     24.546  10.825  89.334  1.00 54.45
ATOM  2250 N   SER  236     17.914  25.370  86.674  0.50 20.48    AC2
ATOM  2251 CA  SER  236     18.176  23.976  86.323  0.50 19.91    AC2
ATOM  2252 CB  SER  236     19.157  23.889  85.166  0.50 18.72    AC2
ATOM  2253 OG  SER  236     19.325  22.538  84.787  0.50 17.70    AC2
ATOM  2254 C   SER  236     18.741  23.171  87.483  0.50 21.62    AC2
ATOM  2255 O   SER  236     19.744  23.549  88.075  0.50 20.94    AC2
ATOM  2256 N   SER  247     25.235  21.608  79.357  0.50 19.68    AC2
ATOM  2257 CA  SER  247     25.203  22.865  78.619  0.50 20.48    AC2
ATOM  2258 CB  SER  247     26.051  23.917  79.337  0.50 19.95    AC2
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ATOM	2259	OG	SER	247	26.032	25.152	78.637	0.50	20.60	AC2
ATOM	2260	C	SER	247	25.725	22.638	77.203	0.50	20.84	AC2
ATOM	2261	O	SER	247	25.203	23.202	76.238	0.50	21.05	AC2
ATOM	2262	N	SER	271	7.551	30.448	53.176	0.50	29.97	AC2
ATOM	2263	CA	SER	271	7.680	31.880	53.442	0.50	31.61	AC2
ATOM	2264	CB	SER	271	8.888	32.443	52.695	0.50	32.22	AC2
ATOM	2265	OG	SER	271	8.666	32.395	51.295	0.50	32.71	AC2
ATOM	2266	C	SER	271	6.432	32.648	53.010	0.50	32.99	AC2
ATOM	2267	O	SER	271	6.229	33.796	53.408	0.50	34.05	AC2
ATOM	2268	N	PRO	319	18.143	-4.099	74.681	0.50	41.20	AC2
ATOM	2269	CD	PRO	319	18.070	-4.311	76.139	0.50	40.63	AC2
ATOM	2270	CA	PRO	319	18.053	-2.673	74.356	0.50	38.50	AC2
ATOM	2271	CB	PRO	319	17.702	-2.038	75.699	0.50	39.26	AC2
ATOM	2272	CG	PRO	319	18.406	-2.938	76.680	0.50	39.94	AC2
ATOM	2273	C	PRO	319	19.321	-2.077	73.756	0.50	35.96	AC2
ATOM	2274	O	PRO	319	20.410	-2.230	74.313	0.50	35.87	AC2
ATOM	2275	N	GLN	343	13.913	5.584	80.085	0.50	18.73	AC2
ATOM	2276	CA	GLN	343	12.714	5.137	79.387	0.50	19.83	AC2
ATOM	2277	CB	GLN	343	11.463	5.365	80.243	0.50	21.34	AC2
ATOM	2278	CG	GLN	343	10.903	4.078	80.837	0.50	26.09	AC2
ATOM	2279	CD	GLN	343	9.539	4.244	81.488	0.50	27.02	AC2
ATOM	2280	OE1	GLN	343	9.412	4.823	82.562	0.50	29.15	AC2
ATOM	2281	NE2	GLN	343	8.508	3.730	80.829	0.50	29.67	AC2
ATOM	2282	C	GLN	343	12.545	5.813	78.025	0.50	19.53	AC2
ATOM	2283	O	GLN	343	12.317	5.141	77.022	0.50	19.10	AC2
ATOM	2284	N	SER	353	14.027	4.461	65.783	0.50	19.97	AC2
ATOM	2285	CA	SER	353	15.191	3.950	65.107	0.50	20.43	AC2
ATOM	2286	CB	SER	353	16.391	4.058	66.033	0.50	20.57	AC2
ATOM	2287	OG	SER	353	17.540	4.234	65.262	0.50	19.64	AC2
ATOM	2288	C	SER	353	15.054	2.524	64.574	0.50	21.08	AC2
ATOM	2289	O	SER	353	15.234	2.291	63.378	0.50	21.51	AC2
ATOM	2290	N	ARG	392	0.696	20.186	53.122	0.50	19.50	AC2
ATOM	2291	CA	ARG	392	0.935	18.822	53.549	0.50	19.96	AC2
ATOM	2292	CB	ARG	392	0.325	18.551	54.925	0.50	19.99	AC2
ATOM	2293	CG	ARG	392	0.603	17.129	55.384	0.50	19.08	AC2
ATOM	2294	CD	ARG	392	0.140	16.884	56.805	0.50	19.85	AC2

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ATOM  2295 NE  ARG  392     -1.315  16.885  56.925  0.50 19.23      AC2
ATOM  2296 CZ  ARG  392     -1.962  16.577  58.046  0.50 21.63      AC2
ATOM  2297 NH1 ARG  392     -1.283  16.242  59.138  0.50 19.92      AC2
ATOM  2298 NH2 ARG  392     -3.289  16.611  58.086  0.50 22.19      AC2
ATOM  2299 C   ARG  392      0.338  17.878  52.501  0.50 19.95      AC2
ATOM  2300 O   ARG  392      0.940  16.867  52.149  0.50 20.64      AC2
ATOM  2301 N   SER  431      9.466  14.172  75.955  0.50 16.96      AC2
ATOM  2302 CA  SER  431     10.735  14.900  76.047  0.50 17.25      AC2
ATOM  2303 CB  SER  431     11.346  15.109  74.659  0.50 17.09      AC2
ATOM  2304 OG  SER  431     10.765  16.211  73.998  0.50 16.93      AC2
ATOM  2305 C   SER  431     10.466  16.249  76.719  0.50 17.71      AC2
ATOM  2306 O   SER  431     11.267  16.716  77.521  0.50 17.14      AC2
END
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Table 2:

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bdrxra      ----FNEEMPVEKILDAELAV-------------EPKTEAYME---------------
murxra      ----ANEDMPVEKILEAELAV-------------EPKTETYVE---------------
rnrxra      ----ANEDMPVEKILEAELAV-------------EPKTETYVE---------------
horxra      ----ANEDMPVERILEAELAV-------------EPKTETYVE---------------
xlrxra      ----ANEDMPVEKILEAEHAV-------------EPKTETYTE---------------
surxrb      ------------------------------------------------------------
aeuspa      -----VRDVTIERIHEAEQLS-----E--------QKSGDNAIPYLR-------------
dmusp       MTNSVSRDFSIERIIEAEQRA-----E--------TQCGDRALTFLR-------------
horxrb      ----APEEMPVDRILEAELAV-------------EQKSDQGVEGP--------------
murxrb      ----APEEMPVDRILEAELAV-------------EQKSDQGVEGP--------------
rnrxrb      ----APEEMPVDRILEAELAV-------------EQKSDQGVEGP--------------
xlrxrbb     ----INEEMPVEKILEAELAV-------------EQKSDQSLE----------------
xlrxrba     ----INEEMPVEKILEAELAV-------------EQKSDQSLE----------------
murxrg      ----SHEDMPVERILEAELAV-------------EPKTESYGD----------------
horxrg      ----GHEDMPVERILEAELAV-------------EPKTESYGD----------------
garxrg      ----GSEDMPVERILEAELAV-------------EPKTEAYSD----------------
xlrxrg      ----TSEEMPVERILEAELAV-------------DPKIEAFGD----------------
pmrxr       ----PNDDMPVDKILEAELIS-------------DPKVEQVVP----------------
lmrxr       ----LHTDMPVERILEAEKRV-------------E------------------------
smrxr       ---TDLPNLTLRCLLSAELSM-------------DPKLAVSERG----------------
amusp       ----LHSDMPIERILEAEKRV-------------ECKMEQQGN----------------
tmusp       ----MQAEMPLDRIIEAEKRI-------------ECTPAGGSG----------------
aarxr       ---GAPPEMPLERILEAELRV-------------ESQTGTLSES----------------
aarxr2      --P-GSPDMPLERILEAEMRV-------------EQPAPSVLAQ----------------
uprxr       ----AISDMPIASIREAELSV-------------DPIDEQPLDQGVRLQVPLAPPDSEK
cfusp       --VQVSDELSIERLTEMESLV------ADPSEE------FQFLR----------------
msusp       -----VQELSIERLLEIESLV------ADPPEE------FQFLR----------------
bmusp       -----VQELSIERLLELEALV------ADSAEE------LQILR----------------
ctusp       --NGPGRDITVERLMEADQMS------EARCGDKS----IQYLR---------V------
uspx        ---AAAQELSIERLLEMESLVAAAAEE------------FQFLR----------------
rxrmin      -ASSANEDMPVEKILEAELAV-------------EPKTETYVE----------------


bdrxra      ---------SSM---SNSTNDPVTNICQAADKQLFTLVEWAKRIPHFSDL---PLDDQVI
murxra      ---------ANMGLNPSSPNDPVTNICQAADKQLFTLVEWAKRIPHFSEL---PLDDQVI
rnrxra      ---------ANMGLNPSSPNDPVTNICQAADKQLFTLVEWAKRIPHFSEL---PLDDQVI
horxra      ---------ANMGLNPSSPNDPVTNICQAADKQLFTLVEWAKRIPHFSEL---PLDDQVI
xlrxra      ---------ANMGLAPNSPSDPVTNICQAADKQLFTLVEWAKRIPHFSDV---PLDDQVI
surxrb      -------------GSGSSPNDPVTNICQAADKQLFTLVEWAKRIPHFSSL---PLDDQVI
aeuspa      --------VGSNSMIPPEYKGAVSHLCQMVNKQIYQLIDFARRVPHFINL---PRDDQVM
dmusp       --------VGPYSTVQPDYKGAVSALCQVVNKQLFQMVEYARMMPHFAQV---PLDDQVI
horxrb      ---------GATGGGGSSPNDPVTNICQAADKQLFTLVEWAKRIPHFSSL---PLDDQVI
murxrb      ---------GATGGGGSSPNDPVTNICQAADKQLFTLVEWAKRIPHFSSL---PLDDQVI
rnrxrb      ---------GATGGGGSSPNDPVTNICQAADKQLFTLVEWAKRIPHFSSL---PLDDQVI
xlrxrbb     --------------GGGSPSDPVTNICQAADKQLFTLVEWAKRIPHFSEL---ALDDQVI
xlrxrba     --------------GGGSPSDPVTNICQDADKQLFTLVEWAKRIPHFSELPELPLDDQVI
murxrg      ------------MNVENSTNDPVTNICHAADKQLFTLVEWAKRIPHFSDL---TLEDQVI
horxrg      ------------MNMENSTNDPVTNICHAADKQLFTLVEWAKRIPHFSDL---TLEDQVI
garxrg      ------------VNTESSTNDPVTNICHAADKQLFTLVEWAKRIPHFSDL---TLEDQVI
xlrxrg      ------------AGLPNSTNDPVTNICHAADKQLFTLVEWAKRIPYFSDL---PLEDQVI
pmrxr       -------------FEQVNENDPVSNICKAADRQLVTLVEWAKRIPHFSSL---PLEDQVI
lmrxr       -------------------------CKAENQVEYELVEWAKHIPHFTSL---PLEDQVL
smrxr       -----EAIYEDIPGDDDTGLHPLTIICQSIEQQLPRIVNWARQLPVFSSVY-LSFDDQFC
amusp       ------------------YENAVSHICNATNKQLFQLVAWAKHIPHFTSL---PLEDQVL
tmusp       --------------GVGEQHDGVNNICQATNKQLFQLVQWAKLIPHFTSL---PMSDQVL
aarxr       ---------------AQQQDPVSSICQAADRQLHQLVQWAKHIPHFEEL---PLEDRMV
aarxr2      -------------TAASGRDPVNSMCQAAP-PLHELVQWARRIPHFEEL---PIEDRTA
uprxr       CSFTLPFHPVSEVSCANPLQDVVSNICQAADRHLVQLVEWAKHIPHFTDL---PIEDQVV
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cfusp      --------VGPDSNVPPRYRAPVSSLCQIGNKQIAALVVWARDIPHFGQL---ELDDQVV
msusp      --------VGPESGVPAKYRAPVSSLCQIGNKQIAALVVWARDIPHFGQL---ELEDQIL
bmusp      --------VGPESGVPAKYRAPVSSLCQIGNKQIAALIVWARDIPHFGQL---EIDDQIL
ctusp      --------AASNTMIPPEYRAPVSAICAMVNKQVFQHMDFCRRLPHFTKL---PLNDQMY
uspx       --------VGPDSNVPPKFRAPVSSLCQIGNKQIAALVVWARDIPHFSQL---EMEDQIL
rxrmin     ---------ANMGLNPSSPNDPVTNICQAADKQLFTLVEWAKRIPHFSEL---PLDDQVI
                                     *          : :.: :* * .:     .*:

bdrxra     LLRAGWNELLIASFSHRSVTVKDG--------------------------ILLATGLHVH
murxra     LLRAGWNELLIASFSHRSIAVKDG--------------------------ILLATGLHVH
rnrxra     LLRAGWNELLIASFSHRSIAVKDG--------------------------ILLATGLHVH
horxra     LLRAGWNELLIASFSHRSIAVKDG--------------------------ILLATGLHVH
xlrxra     LLRAGWNELLIASFSHRSIAVKDG--------------------------ILLATGLHVH
surxrb     LLRAGWNELLIASFSHRSIDVRDG--------------------------ILLATGLHVH
aeuspa     LLRCGWNEMLIAAVAWRSMEYIETER----------SSDGSRITVRQPQLMCLGPNFTLH
dmusp      LLKAAWIELLIANVAWCSIVSLDDGGGGGGGLGHDGSFERRSPGLQPQQLFLNQSFSYH
horxrb     LLRAGWNELLIASFSHRSIDVRDG--------------------------ILLATGLHVH
murxrb     LLRAGWNELLIASFSHRSIDVRDG--------------------------ILLATGLHVH
rnrxrb     LLRAGWNELLIASFSHRSIDVRDG--------------------------ILLATGLHVH
xlrxrbb    LLRAGWNELLIASFSHRSISVKDG--------------------------ILLATGLHVH
xlrxrba    LLRAGWNELLIASFSHRSISEKDG--------------------------ILLATGLHVH
murxrg     LLRAGWNELLIASFSHRSVSVQDG--------------------------ILLATGLHVH
horxrg     LLRAGWNELLIASFSHRSVSVQDG--------------------------ILLATGLHVH
garxrg     LLRAGWNELLIASFSHRSVSVQDG--------------------------ILLATGLHVH
xlrxrg     LLRAGWNELLIASFSHRSVSVQDG--------------------------ILLATGLHVH
pmrxr      LLRAGWNELLIASFSHRSIDVKDS--------------------------ILLASGLHVH
lmrxr      LLRAGWNELLIAAFSHRSVDVKDG--------------------------IVLATGLTVH
smrxr      LIKAAWPELVLISSAYHSTVIRDG--------------------------LLLSIGRHLG
amusp      LLRAGWNELLIASFSHRSIDVKDG--------------------------IVLATGITVH
tmusp      LLRAGWNELLIAAFSHRSIQAQDA--------------------------IVLATGLTVN
aarxr      LLKAGWNELLIAAFSHRSVDVRDG--------------------------IVLATGLVVQ
aarxr2     LLKAGWNELLIAAFSHRSVAVRDG--------------------------IVLATGLVVQ
uprxr      LLKAGWNELLIASFSHRSMGVEDG--------------------------IVLATGLVIH
cfusp      LIKASWNELLLFAIAWRSMEYLEDER----------ENGDGTRSTTQPQLMCLMPGMTLH
msusp      LIKNSWNELLLFAIAWRSMEYLTDER----------ENVD-SRSTAPPQLMCLMPGMTLH
bmusp      LIKGSWNELLLFAIAWRSMEFLNDER----------ENVD-SRNTAPPQLICLMPGMTLH
ctusp      LLKQSLNELLILNIAYMSIQYVEPDRRNADG---------SLERRQISQQMCLSRNYTLG
uspx       LIKGSWNELLLFAIAWRSMEFLTAAAAS------------------PPQLMCLMPGMTLH
rxrmin     LLRAGWNELLIASFSHRSIAVK--------------------------DGILLATGLHVH
           *:: .  *:::   :  *                                : *  .

bdrxra     RSSAHSAGVGSIFDRVLTELVSKMRDMQMDKTELGCLRAIVLFNPDAKGLSNPSEVEALR
murxra     RNSAHSAGVGAIFDRVLTELVSKMRDMQMDKTELGCLRAIVLFNPDSKGLSNPAEVEALR
rnrxra     RNSAHSAGVGAIFDRVLTELVSKMRDMQMDKTELGCLRAIVLFNPDSKGLSNPAEVEALR
horxra     RNSAHSAGVGAIFDRVLTELVSKMRDMQMDKTELGCLRAIVLFNPDSKGLSNPAEVEALR
xlrxra     RNSAHSAGVGAIFDRVLTELVSKMRDMQMDKTELGCLRAIVLFNPDSKGLSNPLEVEALR
surxrb     RNSAHSAGVGAIFDRVLTELVSKMRDMRMDKTELGCLRAIILFNPDAKGLSNPSEVEVLR
aeuspa     RNSAQQAGVDTLFDRILCELGIKMKRLDVTRAELGVLKAIILFNPDIRGLKCQKEIDGMR
dmusp      RNSAIKAGVSAIFDRILSELSVKMKRLNLDRRELSCLKAIILYNPDIRGIKSRAEIEMCR
horxrb     RNSAHSAGVGAIFDRVLTELVSKMRDMRMDKTELGCLRAIILFNPDAKGLSNPGEVEILR
murxrb     RNSAHSAGVGAIFDRVLTELVSKMRDMRMDKTELGCLRAIILFNPDAKGLSNPGEVEILR
rnrxrb     RNSAHSAGVGAIFDRVLTELVSKMRDMRMDKTELGCLRAIILFNPDAKGLSNPGEVEILR
xlrxrbb    RNSAHSAGVGAIFDRVLTELVSKMRDMRMDKTELGCLRAIILFNPDAKGLSNPGDVEVLR
xlrxrba    RNSAHSAGVGAIFERVLTELVSKMRDMRMDKTELGCLRAIILFNPDAKGLSNPGDVEVLR
murxrg     RSSAHSRGVGSIFDRVLTELVSKMKDMQMDKSELGCLRAIVLFNPDAKGLSNPSEVETLR
horxrg     RSSAHSAGVGSIFDRVLTELVSKMKDMQMDKSELGCLRAIVLFNPDAKGLSNPSEVETLR
garxrg     RSSAHSAGVGSIFDRVLTELVSKMKDMQMDKSELGCLRAIVLFNPDAKGLSSPSEVESLR
xlrxrg     RSSAHNAGVGSIFDRVLTELVSKMKDMDMDKSELGCLRAIVLFNPDAKGLSNAAEVEALR
pmrxr      RHSAHQAGVGPIFDRVLTELVSKMRDMMMDKTELGCLRAIVLFNPDVKNLSDSAHIESLR
lmrxr      RNSAHQAGVGTIFDRVLTELVAKMREMKMDKTELGCLRSVILFNPEVRGLKSAQEVELLR
smrxr      REVAKSHGLGPLVDRILHELVARFRDLSLQRTELALLRAIILFNPDANGLSSRHRVEAVR
amusp      RNSAQQAGVGTIFDRVLSELVSKMREMKMDRTELGCLRSIILFNPEVRGLKSIQEVTLLR
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tmusp      KTSAHAVGVGNIYDRVLSELVNKMKEMKMDKTELGCLRAIILYNPTCRGIKSVQEVEMLR
aarxr      RHSAHGAGVGAIFDRVLTELVAKMREMKMDRTELGCLLAVVLFNPEAKGLRTCPSGGPEG
aarxr2     RHSAHGAGVGDIFDRVLAELVAKMRDMKMDKTELGCLRAVVLFNPDAKGLRNATRVEALR
uprxr      RSSAHQAGVGAIFDRVLSELVAKMKEMKIDKTELGCLRSIVLFNPDAKGLNCVNDVEILR
cfusp      RNSAQQAGVGAIFDRVLSELSLKMRTLRMDQAEYVALKAIVLLNPDVKGLKNRQEVDVLR
msusp      RNSALQAGVGQIFDRVLSELSLKMRTLRMDQAEYVALKAIILLNPDVKGLKNKPEVVVLR
bmusp      RNSALQAGVGQIFDRVLSELSLKMRSLRMDQAECVALKAIILLNPDVKGLKNKQEVDVLR
ctusp      RNMAVQAGVVQIFDRILSELSVKMKRLDLDATELCLLKSIVVFNPDVRTLDDRKSIDLLR
uspx       RNSALQAGVGQIFDRVLSELSLKMRTLRVDQAEYVALKAIILLNPDVKGLKNRQEVEVLR
rxrmin     RNSAHSAGVGAIFDRVLTELVSKMRDMQMDKTELGCLRAIVLFNPDSKGLSNPAEVEALR
           :  *   *: : :*:* **  ::: : :   *   * :::: **  . :

bdrxra     EKVYASLEGYTKHNYPDQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
murxra     EKVYASLEAYCKHKYPEQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
rnrxra     EKVYASLEAYCKHKYPEQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
horxra     EKVYASLEAYCKHKYPEQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
xlrxra     EKVYASLEAYCKQKYPEQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
surxrb     EKVYASLETYCKQKYPEQQGRFAKLLLRLPALRSIGLKCLEHLFFFKLI-----------
aeuspa     EKIYACLDEHCKQQHPSEDGRFAQLLLRLPALRSISLKCLDHLNFIRLLSDKHLDSFIVE
dmusp      EKVYACLDEHCRLEHPGDDGRFAQLLLRLPALRSISLKCQDHLFLFRITSDRPLEELFLE
horxrb     EKVYASLETYCKQKYPEQQGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
murxrb     EKVYASLETYCKQKYPEQQGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
rnrxrb     EKVYASLETYCKQKYPEQQGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
xlrxrbb    EKVYASLESYCKQKYPDQQGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
xlrxrba    EKVYACLESYCKQKYPDQQGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
murxrg     EKVYATLEAYTKQKYPEQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDSFLME
horxrg     EKVYATLEAYTKQKYPEQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
garxrg     EKVYATLEAYTKQKYPEQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
xlrxrg     EKVYATLESYTKQKYPDQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
pmrxr      EKVYASLEAYCRSKYPDQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDKFLMN
lmrxr      EKVYAALEEYTRTTHPDEPGRFAKLLLRLPSLRSIGLKCLEHLFFFRLIGDVPIDTFLME
smrxr      EQLYSALHSYCTTNQPQDTSRFTKLLLRLPPLRSIASKCLEHLVFVKLAAEDPTSCRLIN
amusp      EKIYGALEGYCRVAWPDDAGRFAKLLLRLPAIRSIGLKCLEYLFFFKMIGDVPIDDFLVE
tmusp      EKIYGVLEEYTRTTHPNEPGRFAKLLLRLPALRSIGLKCSEHLFFFKLIGDVPIDTFLME
aarxr      ESV-SALEEHCRQQYPDQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDNFLLS
aarxr2     EKVYAALEEHCRRHHPDQPGRFGKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDSFLLN
uprxr      EKVYAALEEYTRTTYPDEPGRFAKLLLRLPALRSIGLKCLEYLFLFKLIGDTPLDSYLMK
cfusp      EKMFSCLDDYCRRSRSNEEGRFASLLLRLPALRSISLKSFEHLYFFHLVAEGSISGYIRE
msusp      EKMFSCLDEYVRRSRCAEEGRFAALLLRLPALRSISLKCFEHLYFFHLVADTSIASYIHD
bmusp      EKMFLCLDEYCRRSRGGEEGRFAALLLRLPALRSISLKSFEHLYLFHLVAEGSVSSYIRD
ctusp      SRIYASLDEYCRQKHPNEDGRFAQLLLRLPALRSISLKCLDHLFYFQLIDDKNVENSVIE
uspx       EKMFLCLDEYCRRSRSSEEGRFAALLLRLPALRSISLKSFEHLFFFHLVADTSIAGYIRD
rxrmin     EKVYASLEAYCKHKYPEQPGRFAKLLLRLPALRSIGLKCLEHLFFFKLIGDTPIDTFLME
           . :   *. :       : .**  ******.:***. *. ::*  .::

bdrxra     MLEAPHQIT
murxra     MLEAPHQAT
rnrxra     MLEAPHQTT
horxra     MLEAPHQMT
xlrxra     MLEAPHQMT
surxrb     ---------
aeuspa     MLDMPI---
dmusp      QLEAPPPPG
horxrb     MLEAPHQLA
murxrb     MLEAPHQLA
rnrxrb     MLEAPHQLA
xlrxrbb    MLEAPHQLS
xlrxrba    MLEAPHQLS
murxrg     MLETPLQIT
horxrg     MLETPLQIT
garxrg     MLETPLQVT
xlrxrg     MLETPHQIS
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pmrxr           MLETTSDFP
lmrxr           MLESPSDS-
smrxr           LVEHGVWPI
amusp           MLESRSDP-
tmusp           MLESPADA-
aarxr           MLEAPSDP-
aarxr2          MLEAPADP-
uprxr           MLVDNPNTS
cfusp           ALRNHAPPI
msusp           ALRNHAPSI
bmusp           ALCNHAPPI
ctusp           EFHKLN---
uspx            ALRNGG---
rxrmin          MLEAP----
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